Slides, notes, and exercises at:
https://github.com/cheshyre/nptls-hf

Nuclear structure beyond the mean field

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 6

Matthias Heinz, ORNL

Work supported by:

Recap

- Hartree-Fock solves for **best Slater determinant approximation** $|\Phi_{\mathrm{HF}}\rangle$ to ground state $|\Psi\rangle$
- Computes average potential felt by nucleons
- Gives correct asymptotic $\sim e^{-kr}$ behavior for single-particle wave functions
- $|\Phi_{\mathrm{HF}}\rangle$ gives about 50 % of exact binding energy, and charge radius is approximately correct (within 2-3 %)

What about bigger calculations?

- More clever treatment of symmetries of nuclear forces allows large $e_{\max}$
  - Most important: **Rotational invariance**
  - Two-body matrix elements $\langle (pq)JM_J | V_{NN} | (rs)JM_J \rangle$ are diagonal in J, M_J and independent of M_J
  - Reduces storage cost by 100 to 1000
- Open-source codes available

Miyagi, EPJA **59**, 150 (2023)

  - NuHamil: https://github.com/Takayuki-Miyagi/NuHamil-public
  - imsrg++: https://github.com/ragnarstroberg/imsrg

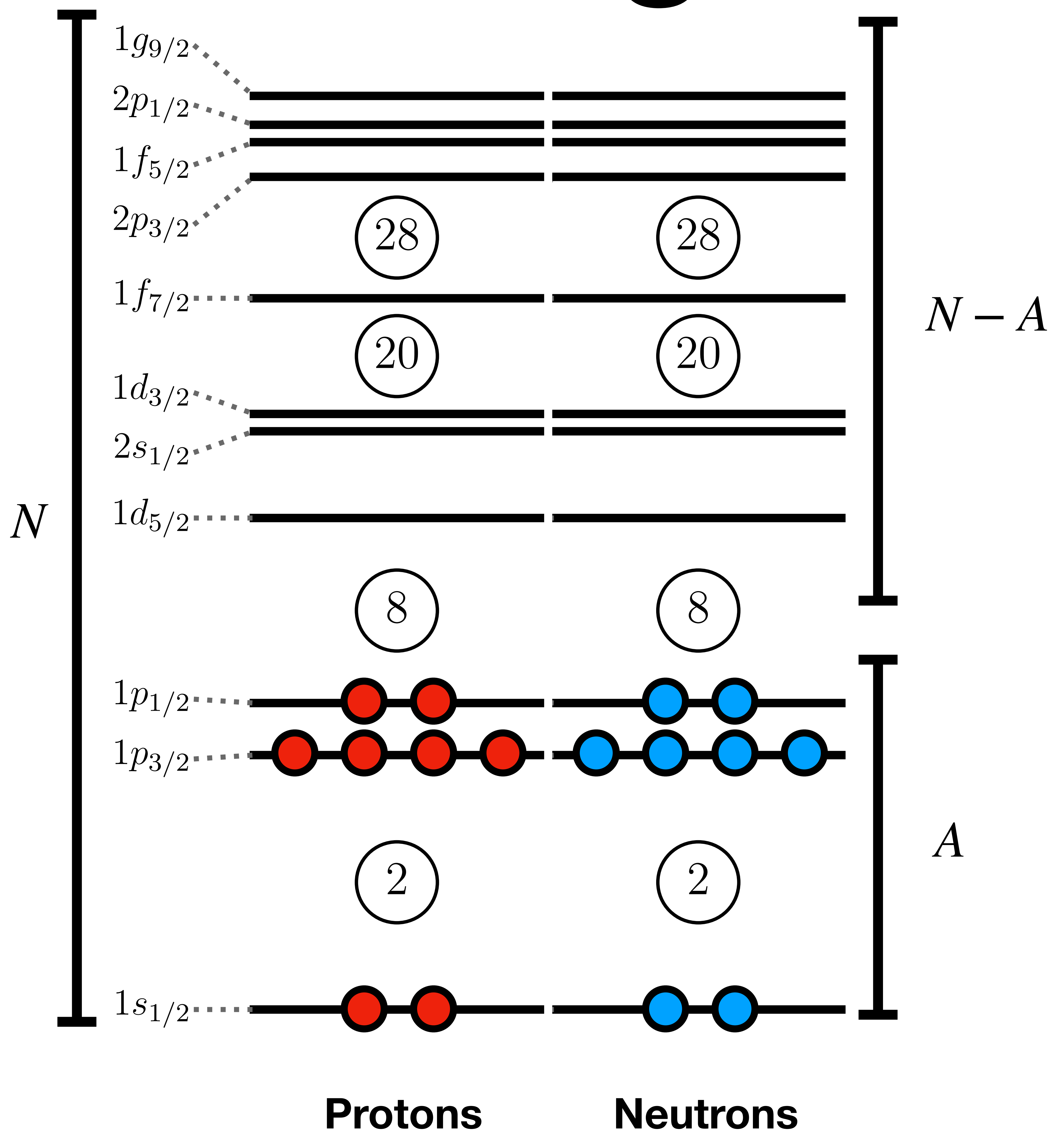
NPTLS-HF repository will be updated to allow you to reach $e_{\max} = 8$!

Today

1. **Ab initio many-body methods** to compute $|\Psi\rangle$
2. **Basis optimization** beyond HF
3. **Deformed nuclei** from Hartree-Fock

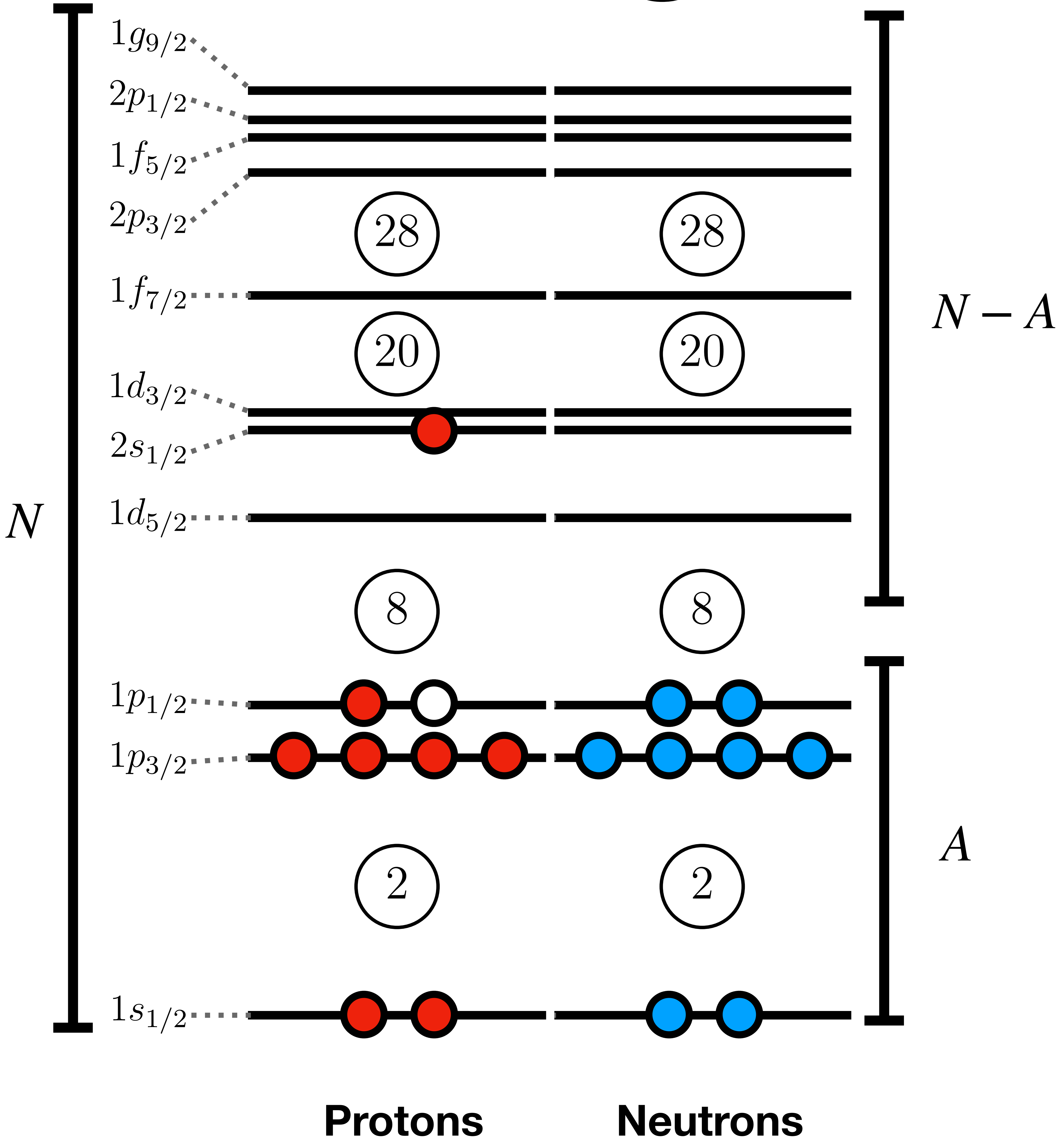
Ab initio many-body methods

Solving the many-body problem



$$|\Phi_{\mathrm{HF}}\rangle \sim \prod_{i=1}^{A} |\phi_i\rangle$$ mean-field reference state

Solving the many-body problem



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$|\Phi_i^a\rangle$ 1p1h excitation ($\binom{A}{1}\binom{N-A}{1}$ states)

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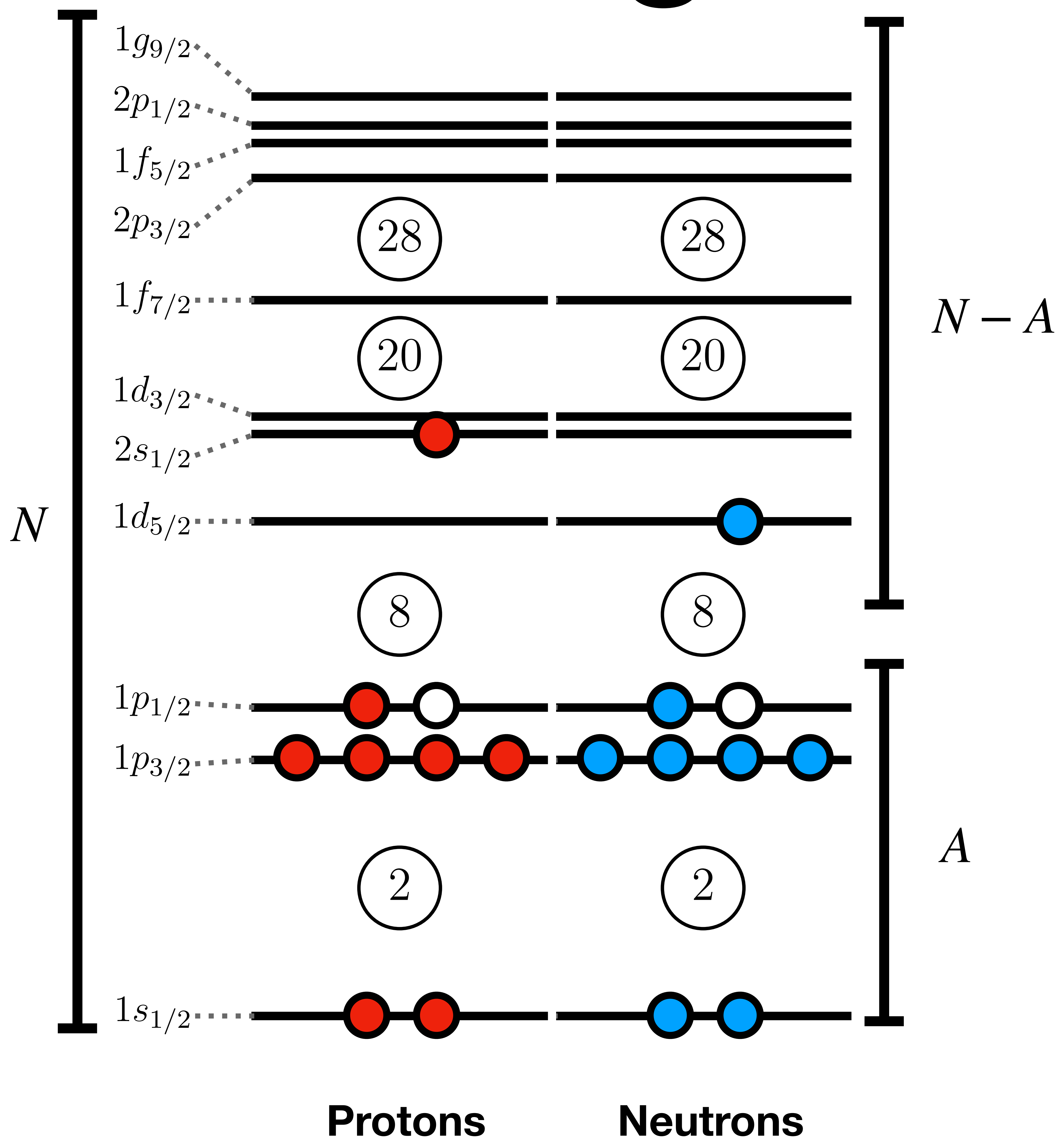

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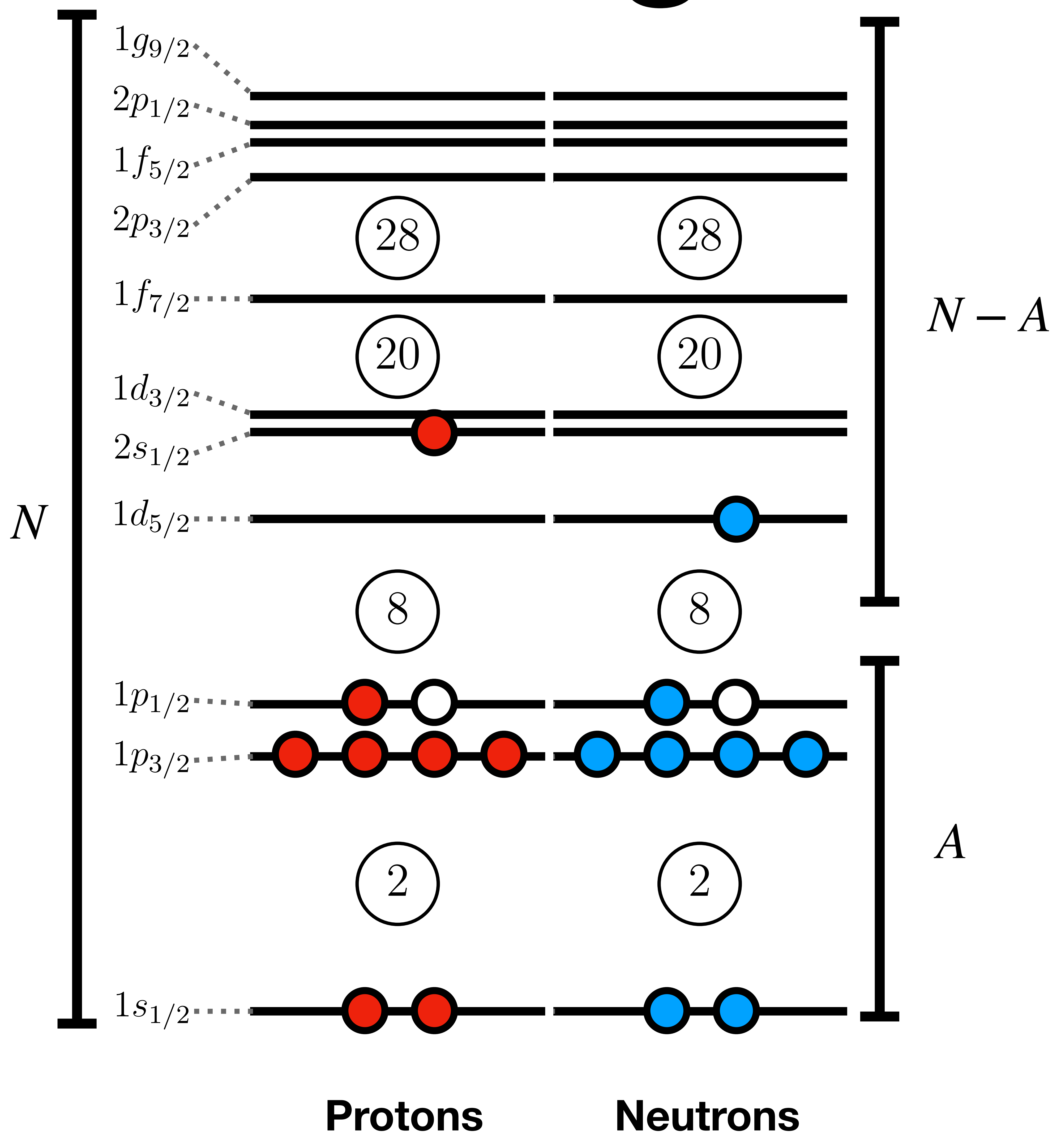

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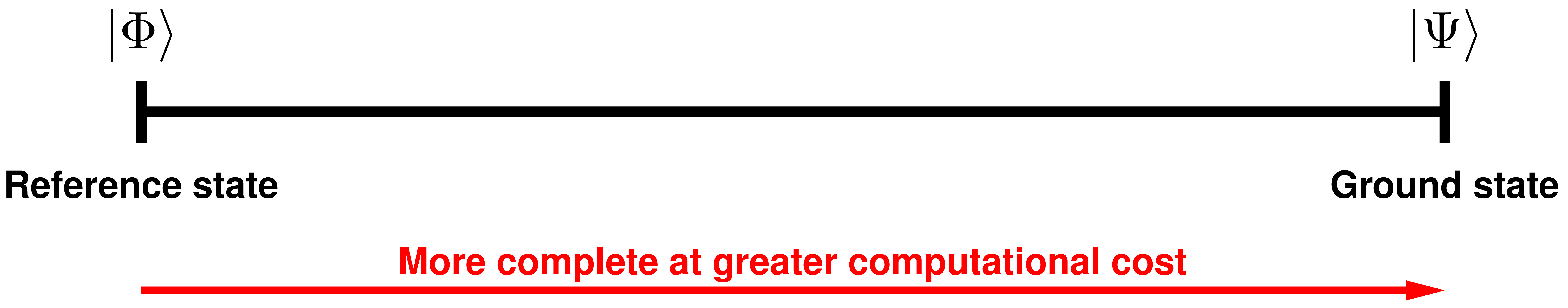
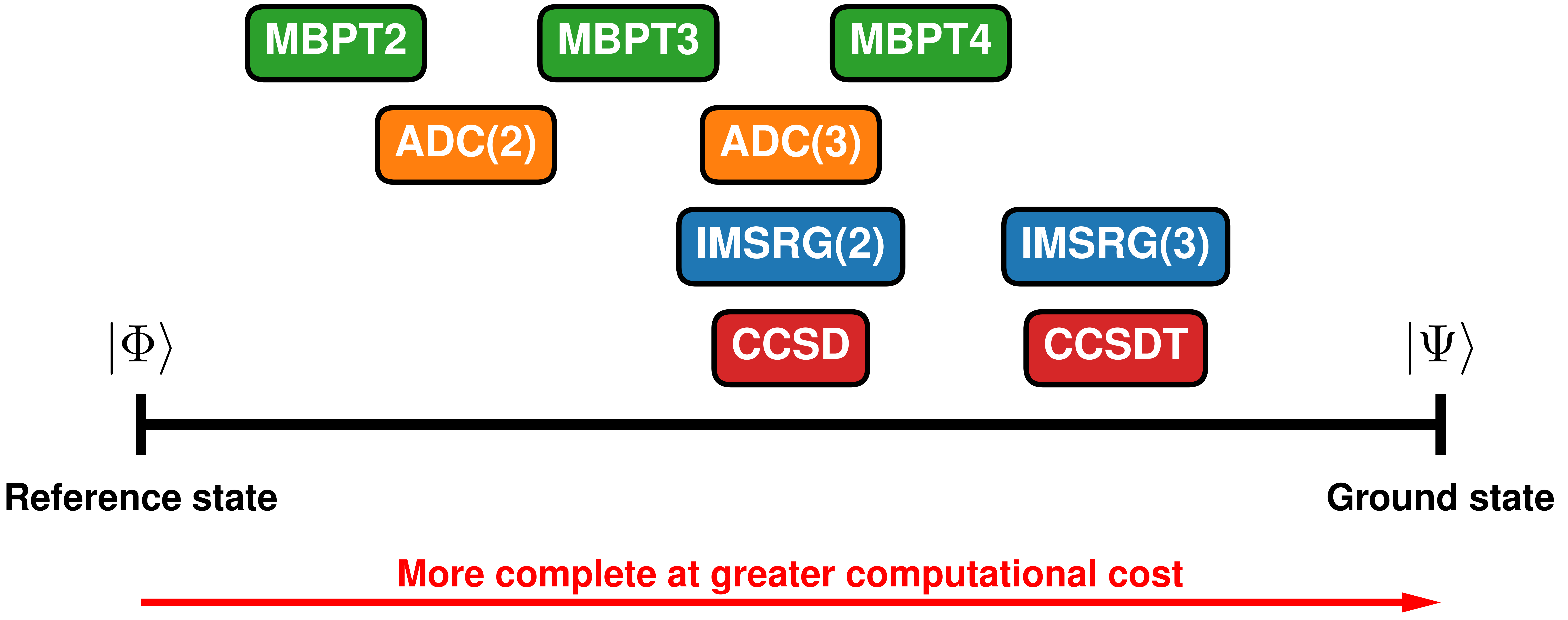
- Scales factorially in A and N

Many-body expansion methods



Many-body expansion methods

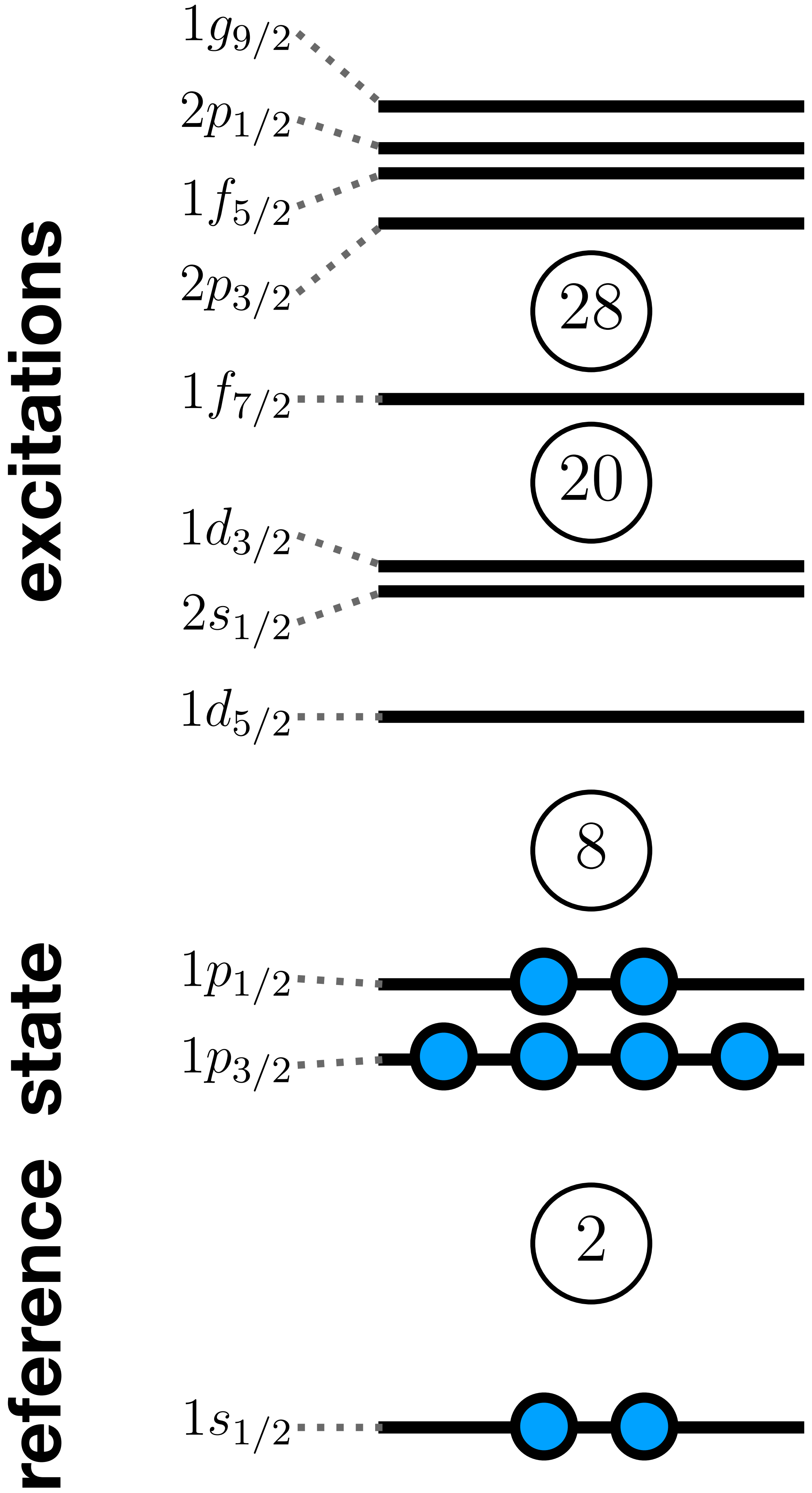


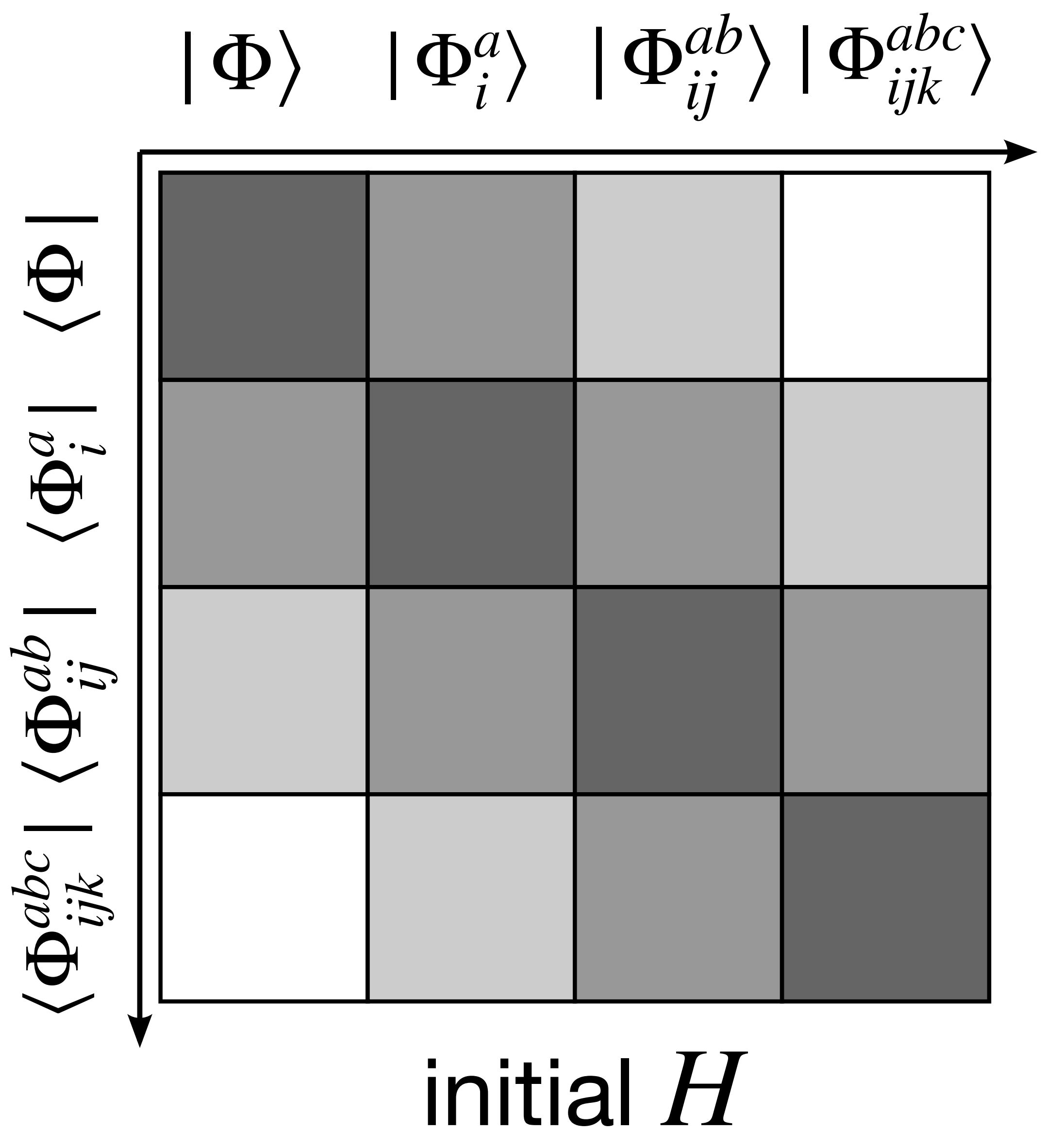
- **Systematically improvable expansion** around reference state $|\Phi_{\mathrm{HF}}\rangle$
- **Tractable computational cost** in larger nuclei
- Approximate many-body solution with **quantifiable uncertainty**

Tsukiyama et al., PRL **106** (2011)
Hergert et al., Phys. Rep. **621** (2016)

The IMSRG

in-medium similarity renormalization group





Tsukiyama et al., PRL **106** (2011)
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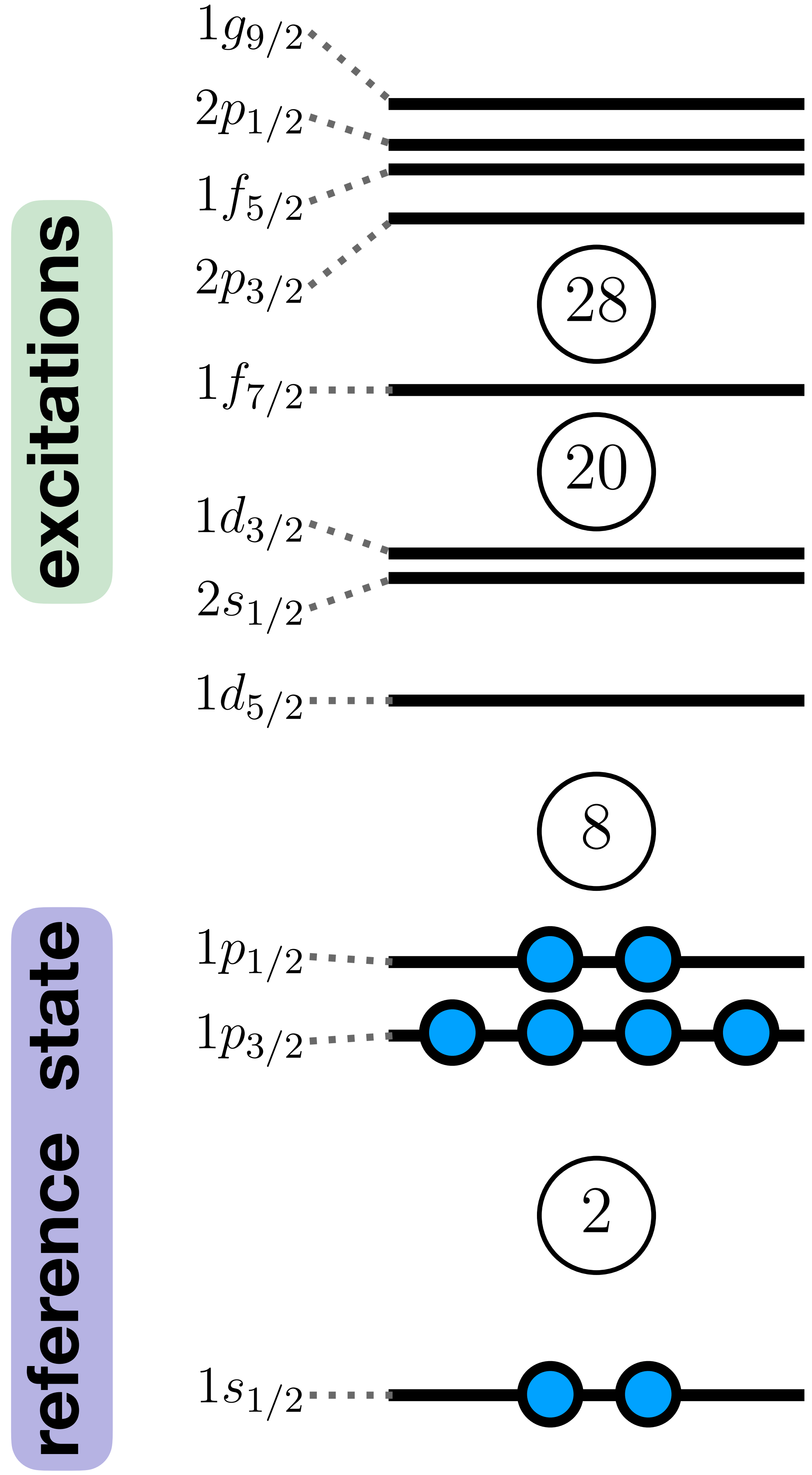

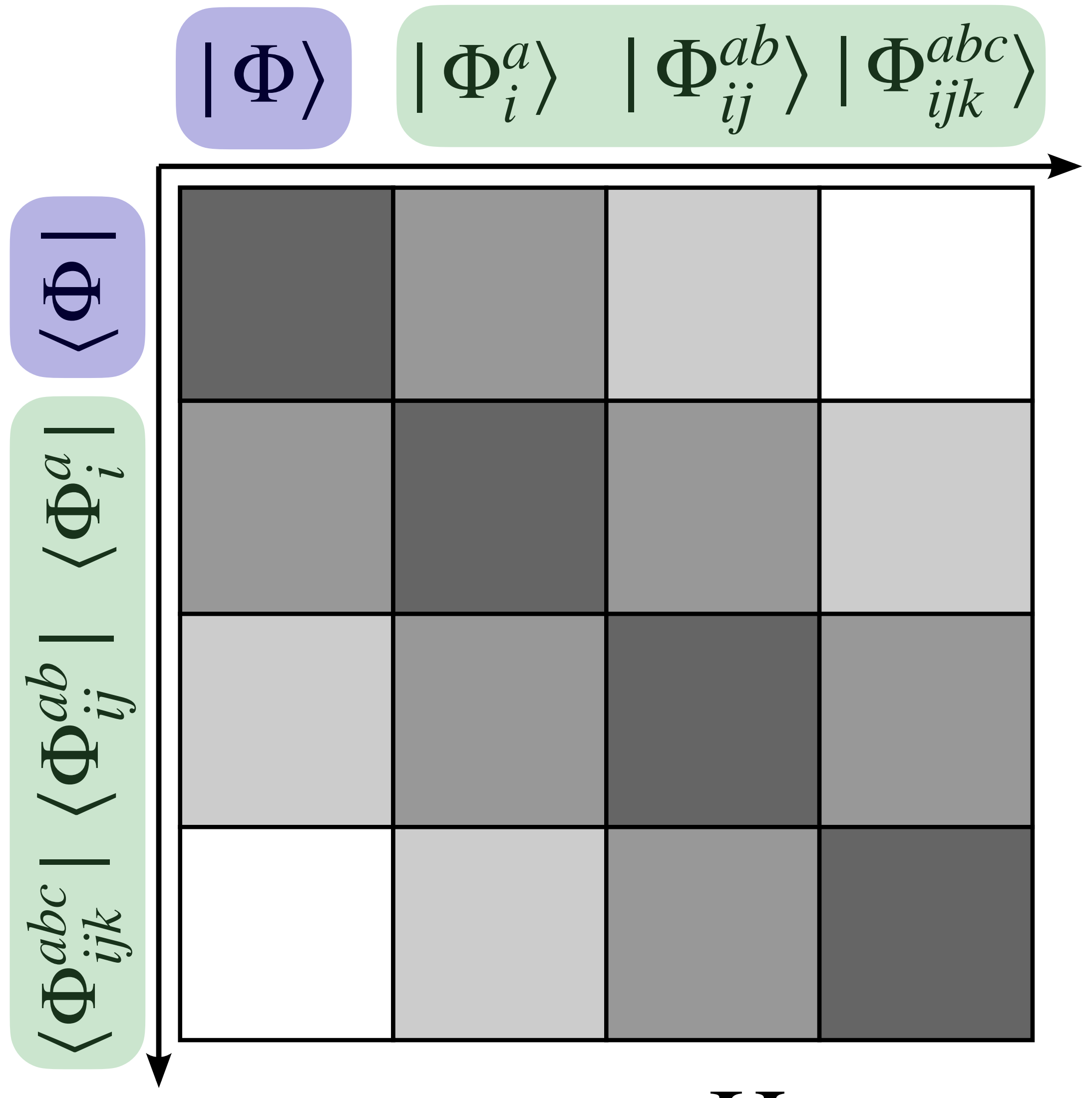

initial H

Tsukiyama et al., PRL **106** (2011)
Hergert et al., Phys. Rep. **621** (2016)

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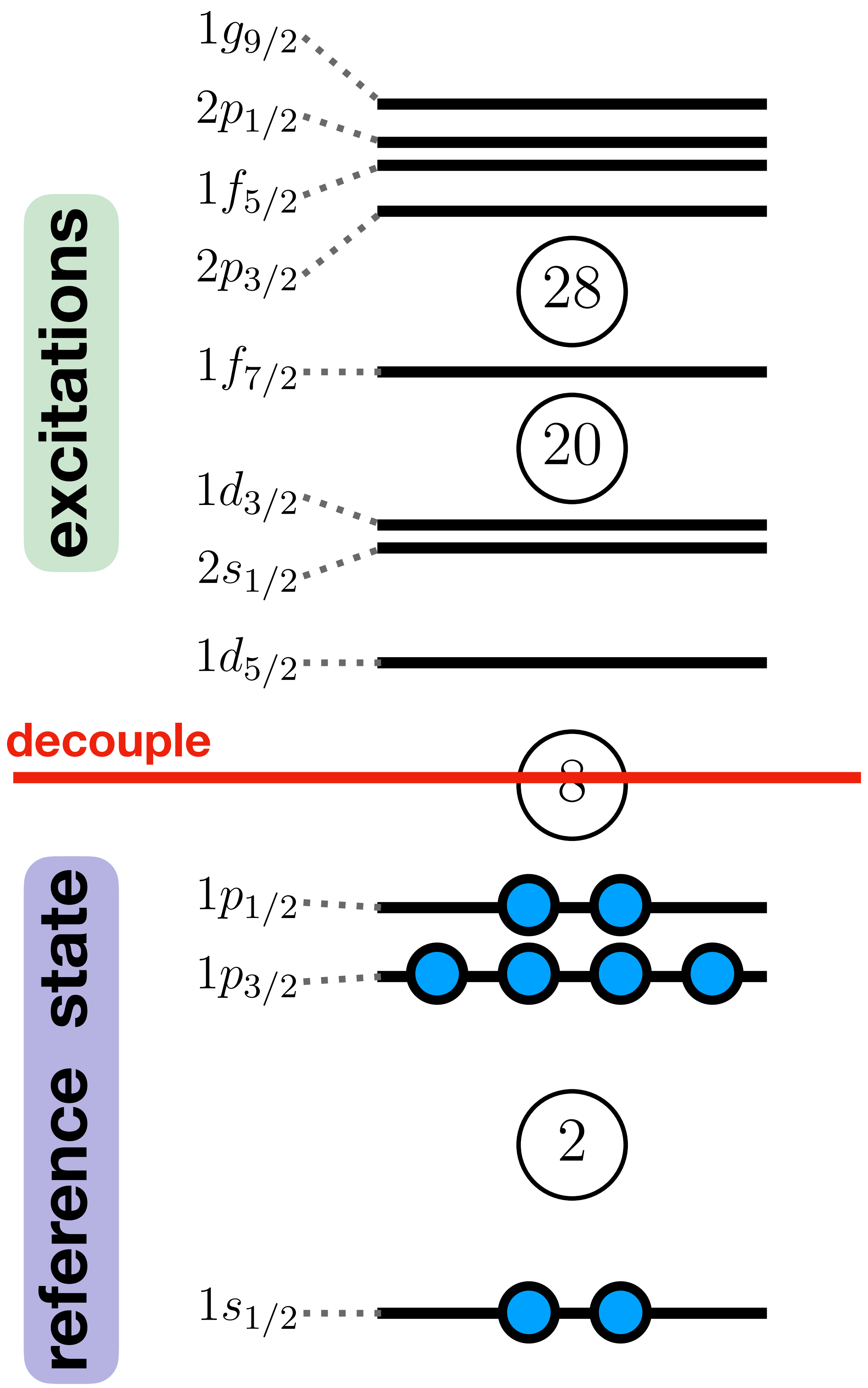

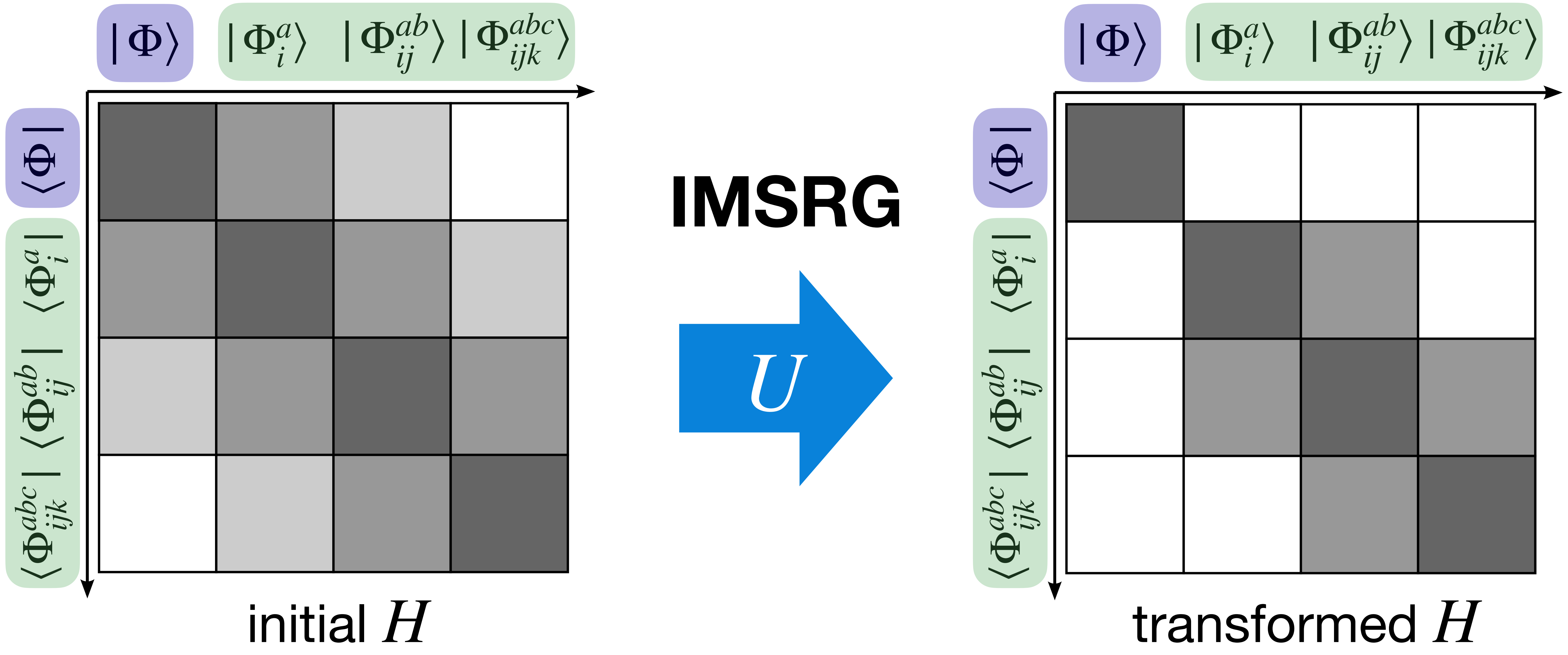

Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations

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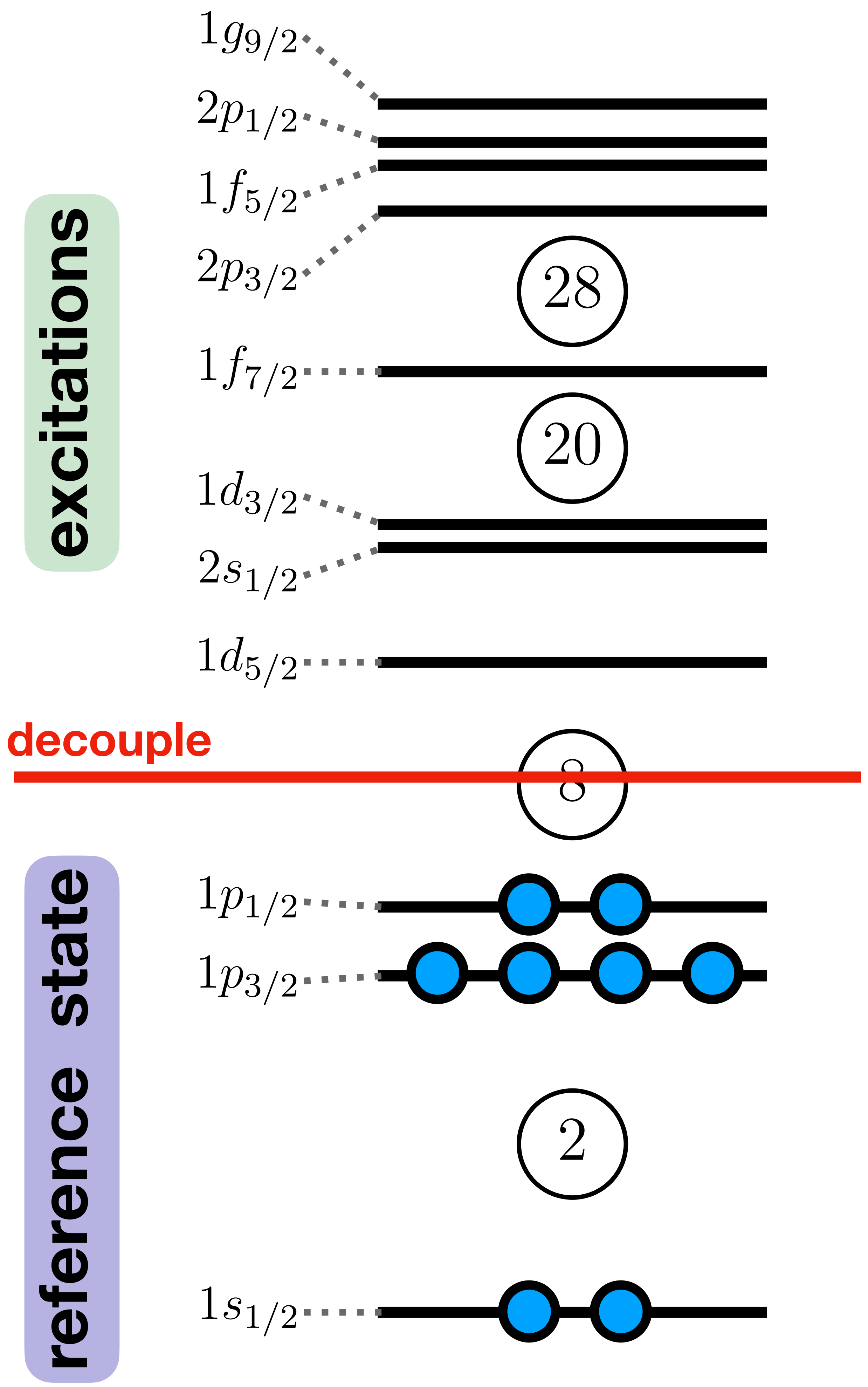
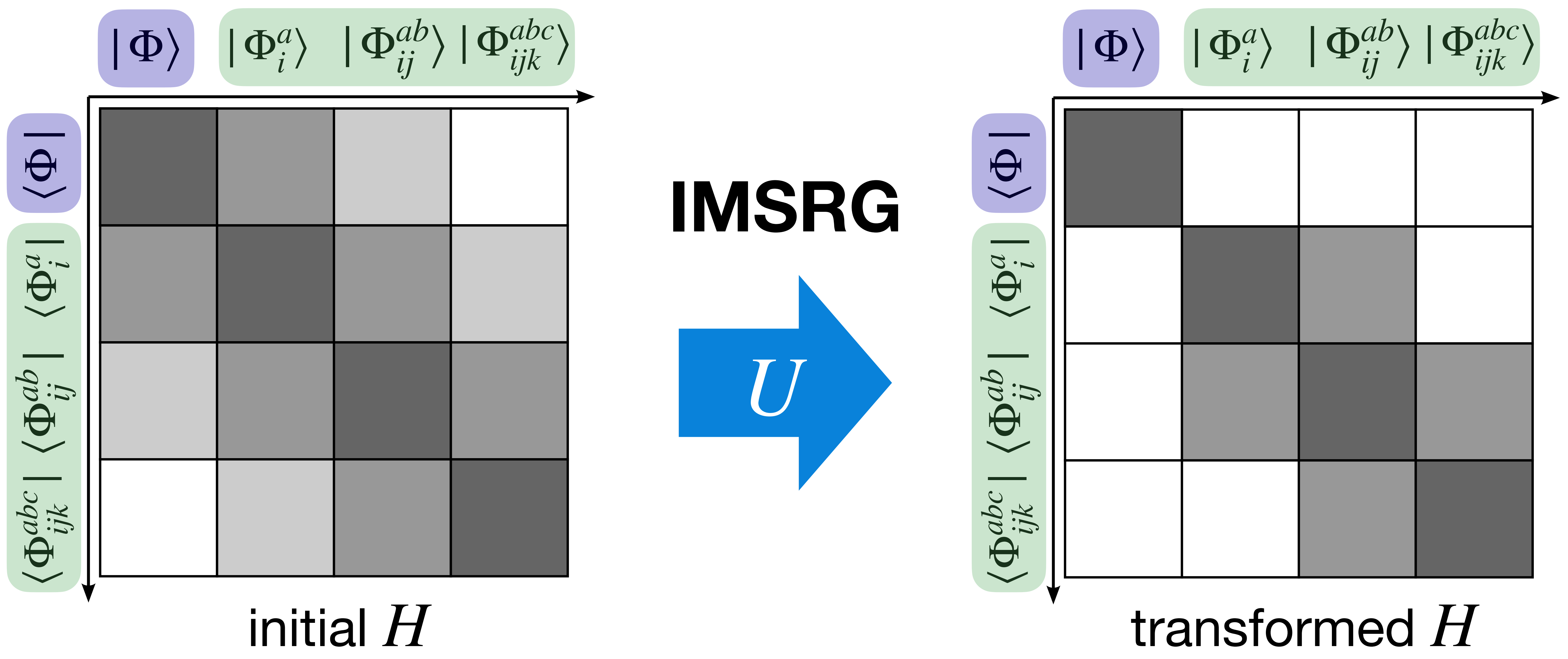




Hergert et al., Phys. Rep. **621** (2016)

- **IMSRG**: Unitary transformation $U = e^{\Omega}$ to decouple reference state from excitations
- Expansion and truncation in **many-body operators**

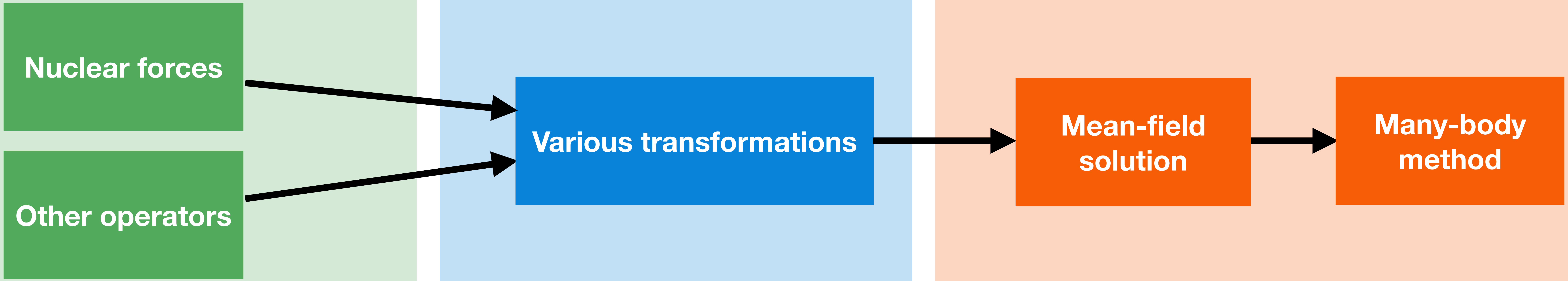
$$U = e^{\Omega} = e^{\Omega_1+\Omega_2+\Omega_3+\dots}$$

MH et al., PRC **103** (2021)

- **IMSRG(3)** for **precision** and **uncertainty quantification**

Ab initio calculation uncertainties

Operator determination | **Basis transformation** | **Many-body calculation**

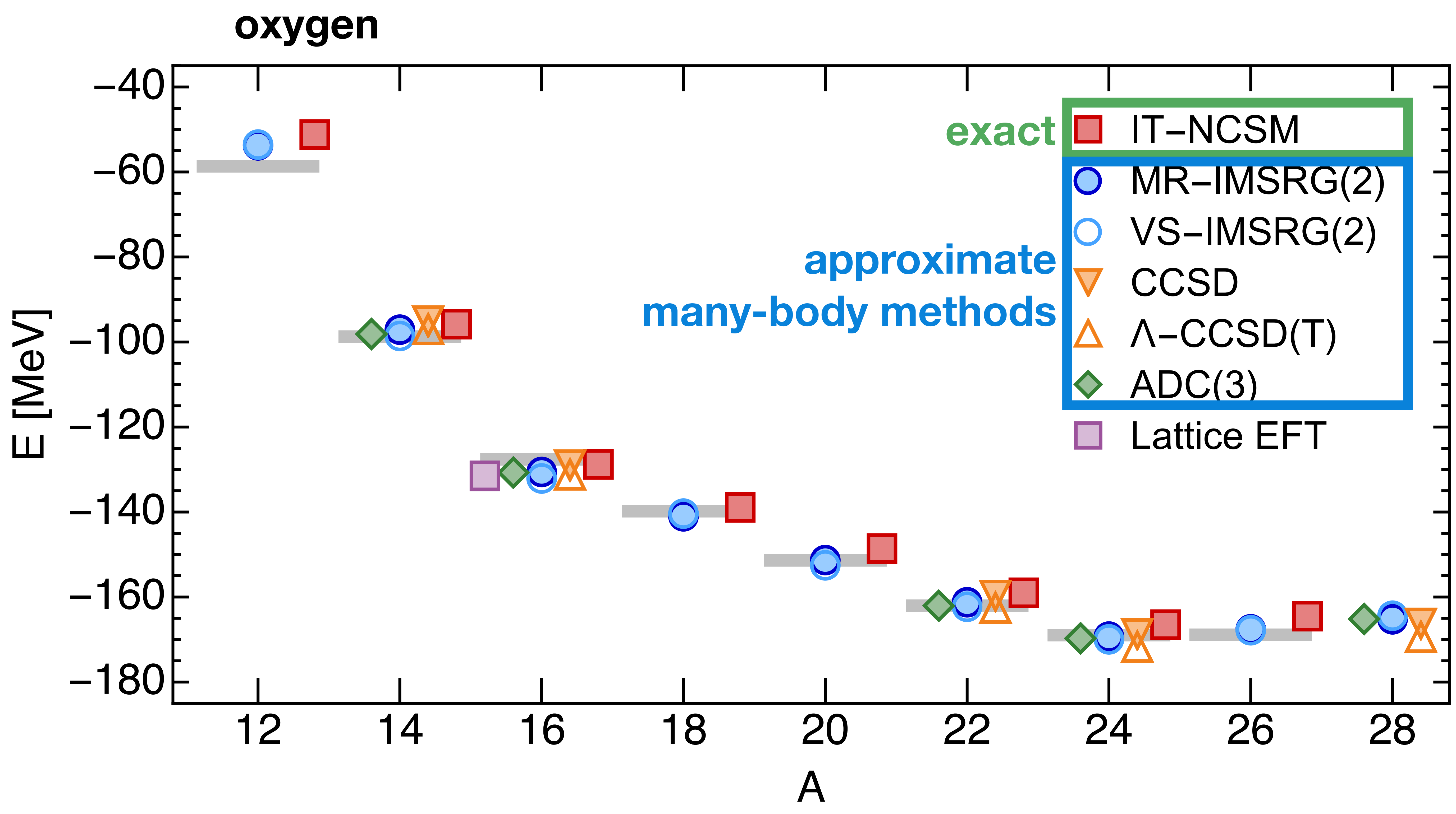


Hamiltonian uncertainty
- **High-order effective theories**

Model-space uncertainty
- **Large basis truncations**

Many-body uncertainty
- **High-order many-body methods**

Many-body consistency in oxygen

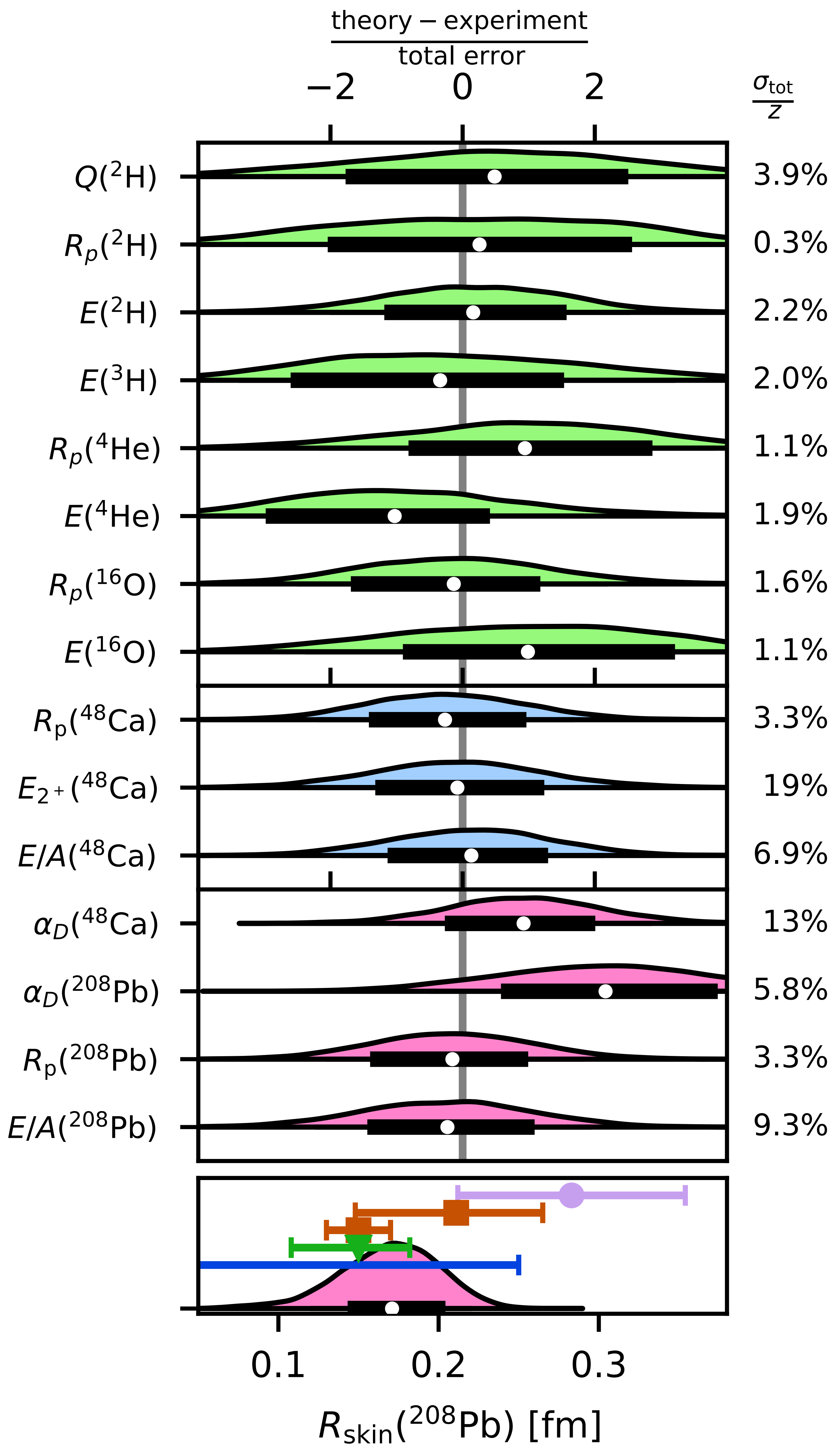


Hergert, Front. Phys. **7** (2020)

- For given Hamiltonian, many-body methods are very consistent
- 1-2% discrepancy to **exact result** due to **many-body approximation**

Various consistent methods to access medium-heavy nuclei available!

First systematic study of ^{208}Pb



Hu et al., Nature Phys. **18** (2022)

History matching:
- Start from 10^9 Hamiltonians
- Compare predictions with experiment and discard "implausible" Hamiltonians
- Final result: 34 different valid choices

Likelihood calibration:
- Assess quality of valid Hamiltonians in calcium-48
- Assign importance weight based on quality

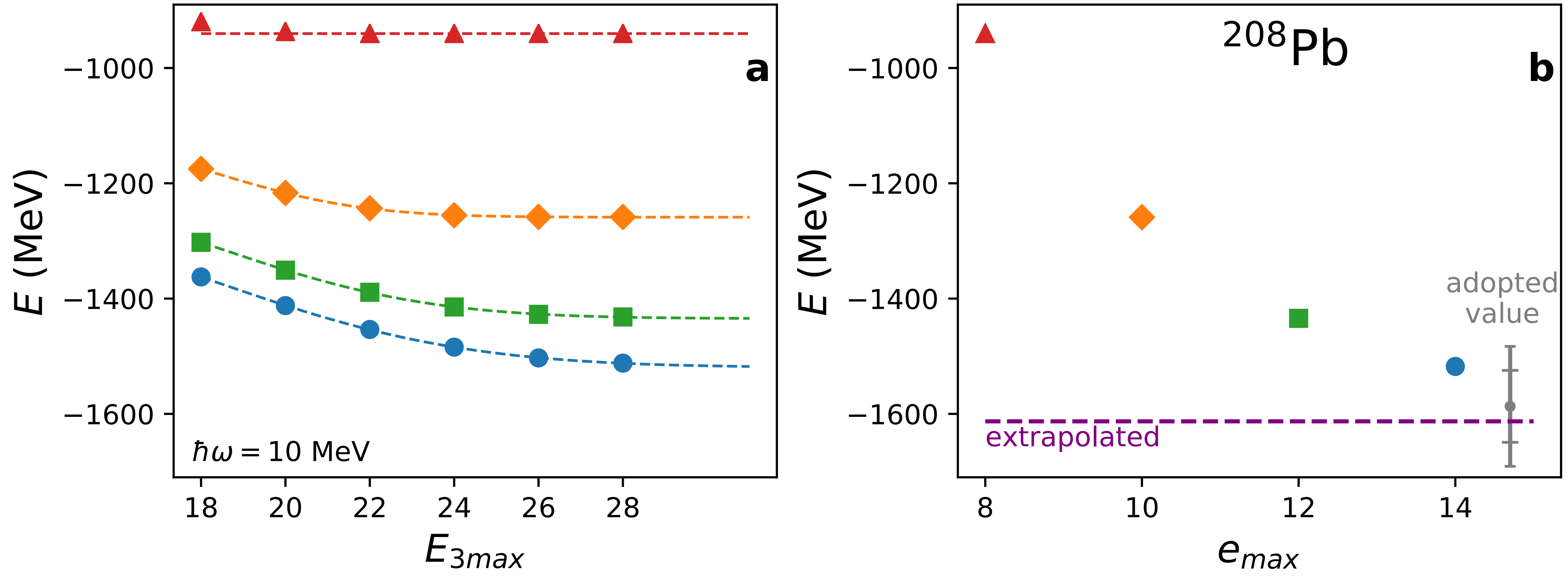
Uncertainty quantified prediction:
- Make many-body prediction using all valid Hamiltonians

$$R_{\text{skin}} = 0.14\text{-}0.20 \text{ fm}$$

Hamiltonian, model space, and method uncertainties accounted for at all stages!

First systematic study of ^{208}Pb

- Convergence of many-body calculation still challenging
- Hamiltonian uncertainties also very large
- Uncertainty quantification methods explicitly take errors into account
- Look at observables where correlated errors cancel?



Hu et al., Nature Phys. **18** (2022)

Basis optimization beyond HF

Natural orbitals basis

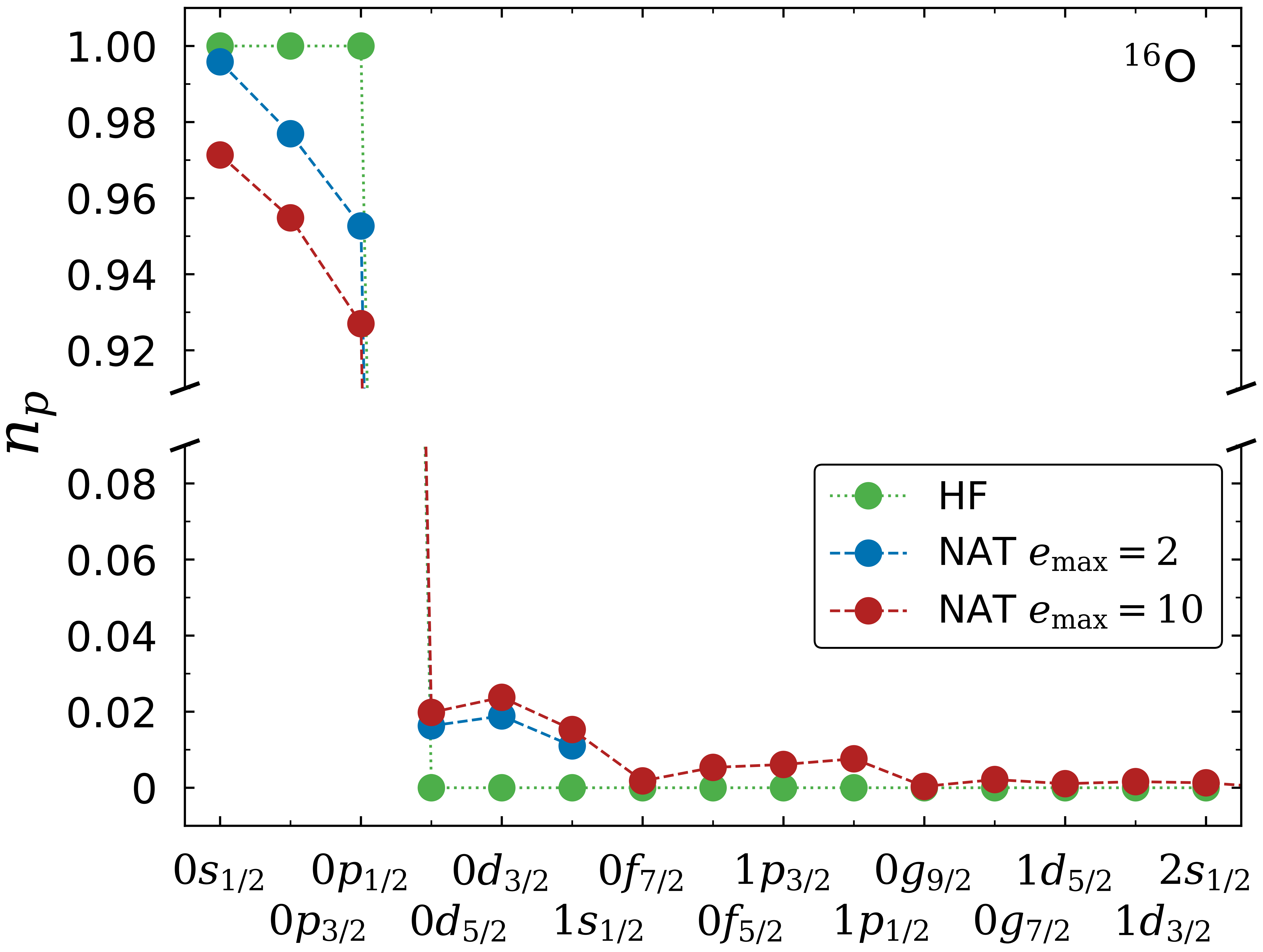
- Natural orbitals are eigenstates of full one-body density matrix

$$\rho_{pq} = \langle \Psi | a_p^\dagger a_q | \Psi \rangle$$

- $|\Phi_{\mathrm{HF}}\rangle$ is leading approximation to $|\Psi\rangle$
- Gives standard diagonal density matrix $\mathrm{diag}(n_p)$
- Can get a better approximation to $|\Psi\rangle$ with perturbation theory

Density matrix beyond HF

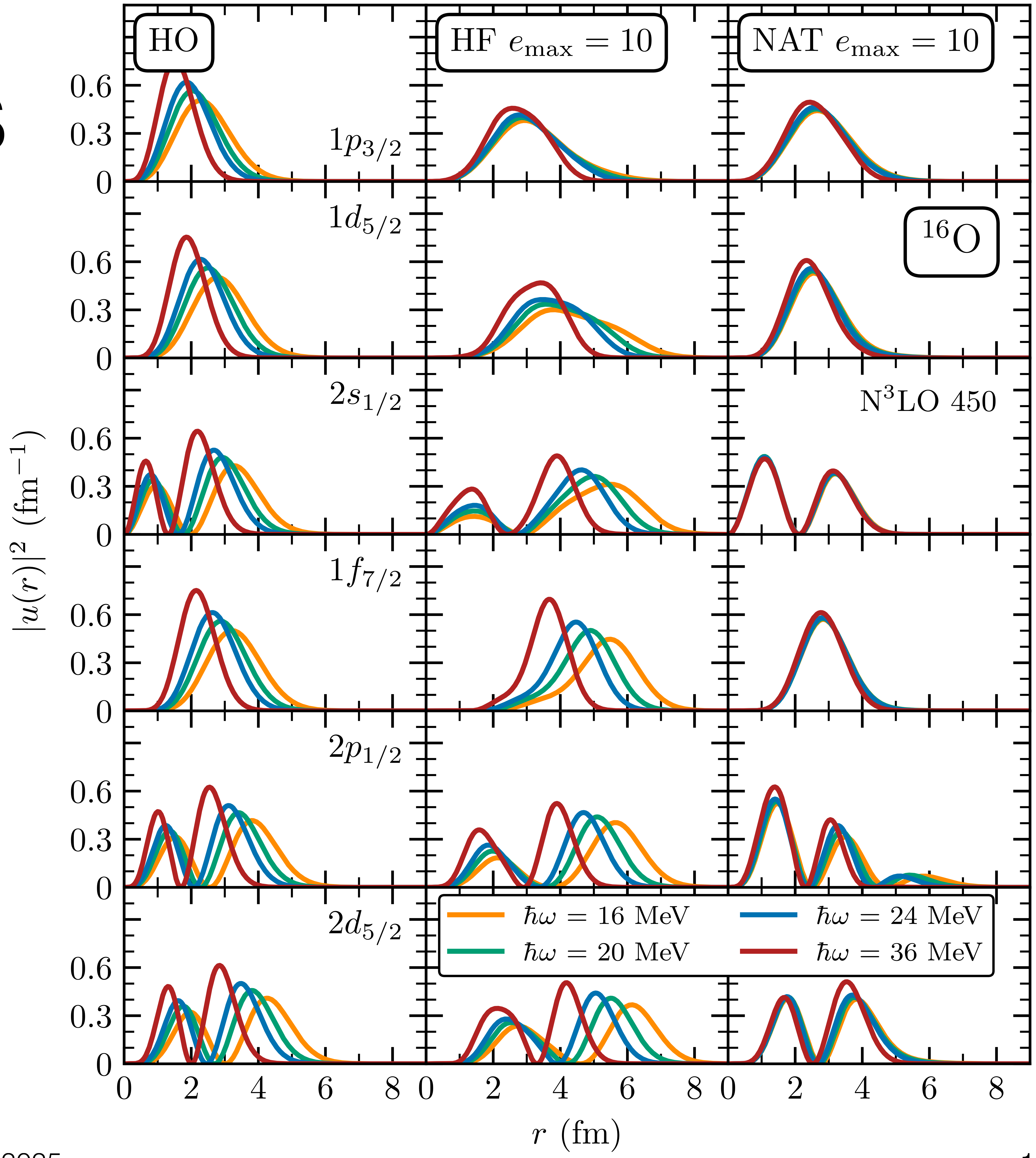
- Beyond HF, $|\Psi_{\text{approx}}\rangle$ is no longer Slater determinant
- Occupation numbers become **"smeared out"** by many-body correlations
- Intuition: the size of the change from HF reflects **importance of state**
- Most important states **near Fermi surface**



Hoppe et al., PRC **103** (2021)

Optimized orbitals

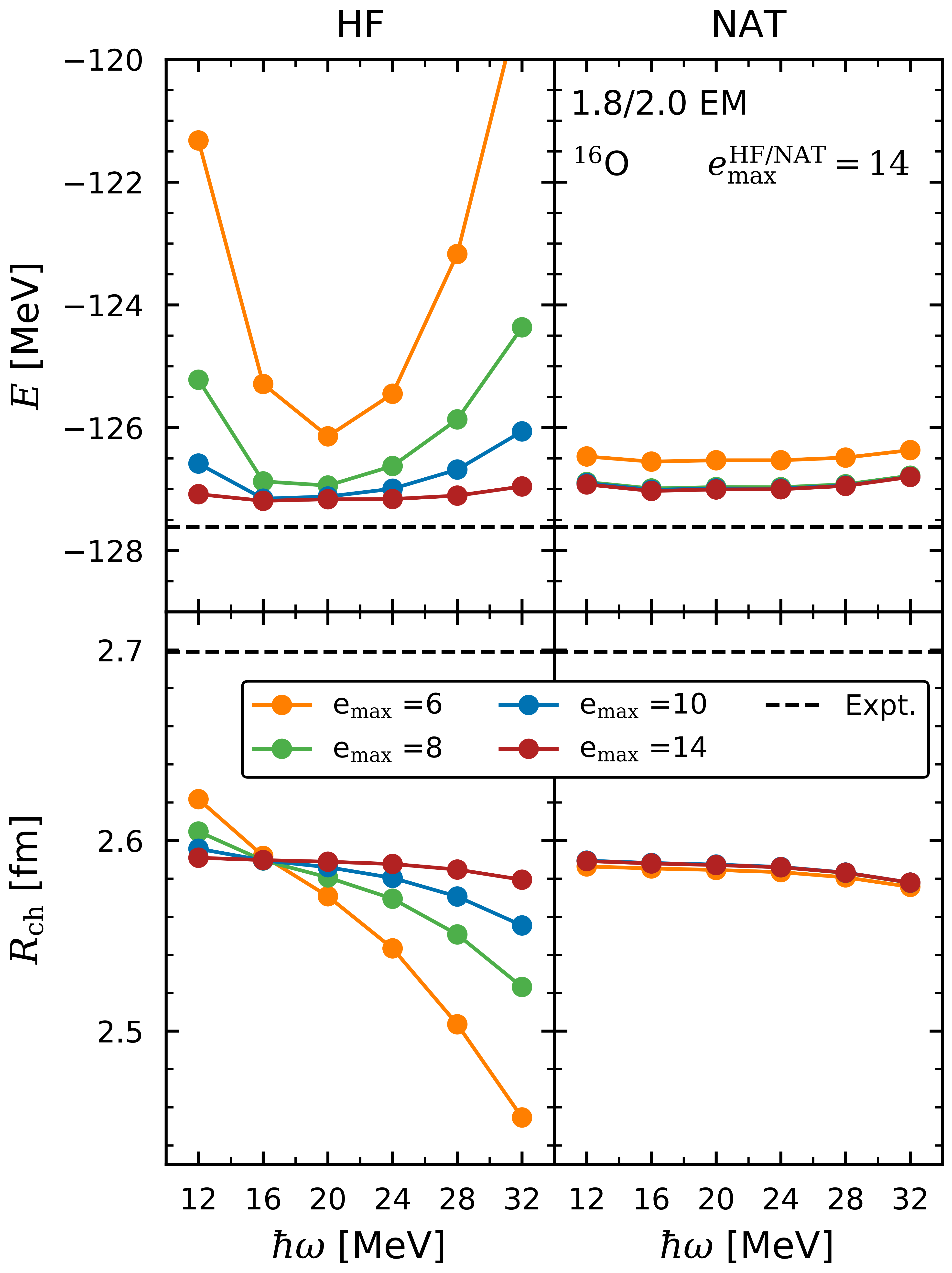
- HF only optimizes occupied states
- NAT (natural orbitals) optimize low-lying unoccupied states as well
- Dependence on $\hbar\omega$ reduced
- Perfect natural orbitals with exact solution $|\Psi\rangle$ would be completely indep. of $\hbar\omega$



Hoppe et al., PRC **103** (2021)

Faster convergence

- NAT basis provides reduced frequency dependence in energies and radii
- Optimized basis can be truncated to smaller $e_{\max}$ and **still give converged results**
- **Really useful to reduce costs of many-body calculation**
- Limit:
  Cannot do better than HF starting basis, but can achieve same result in smaller $e_{\max}$



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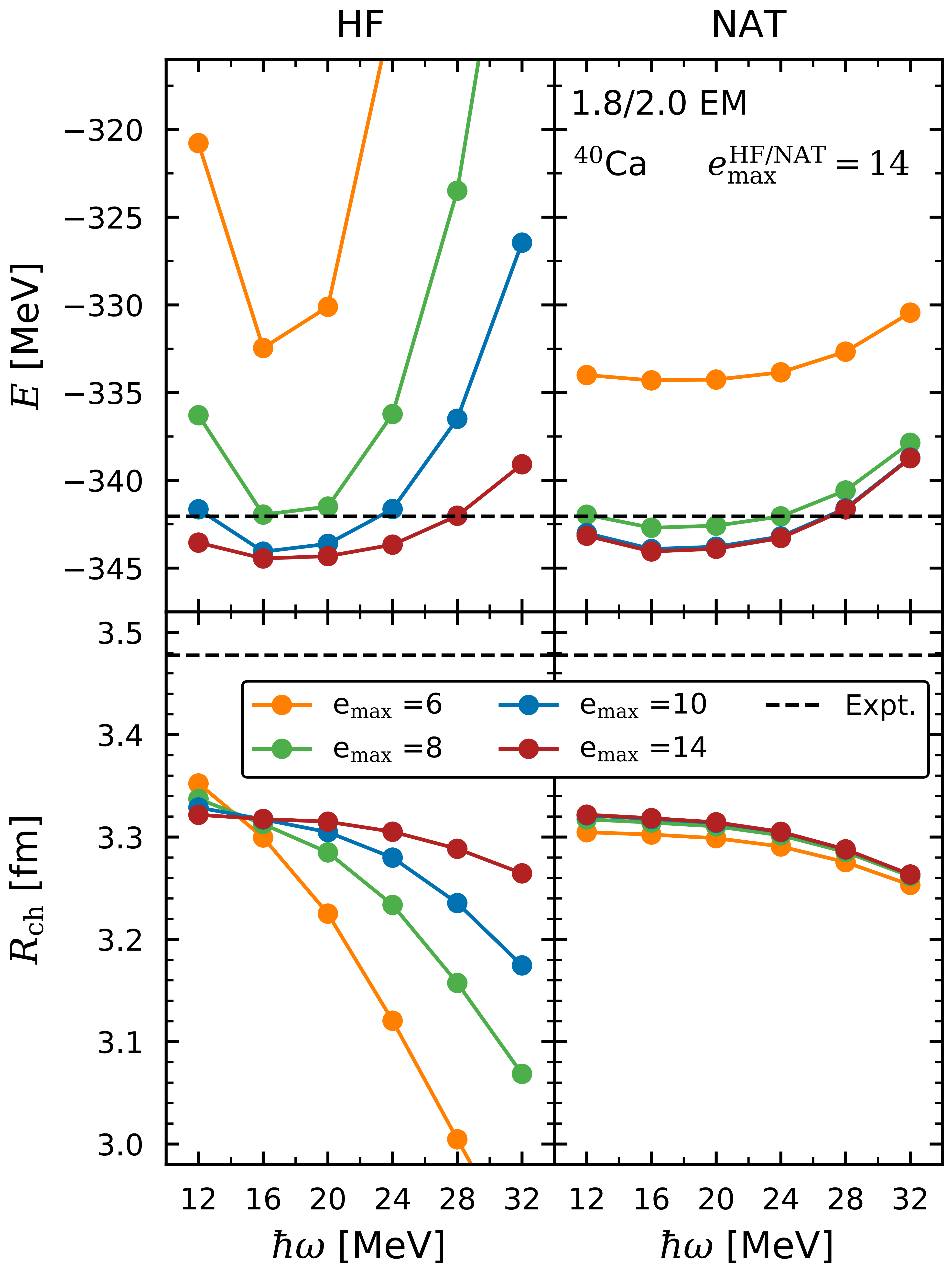

Hoppe et al., PRC **103** (2021)

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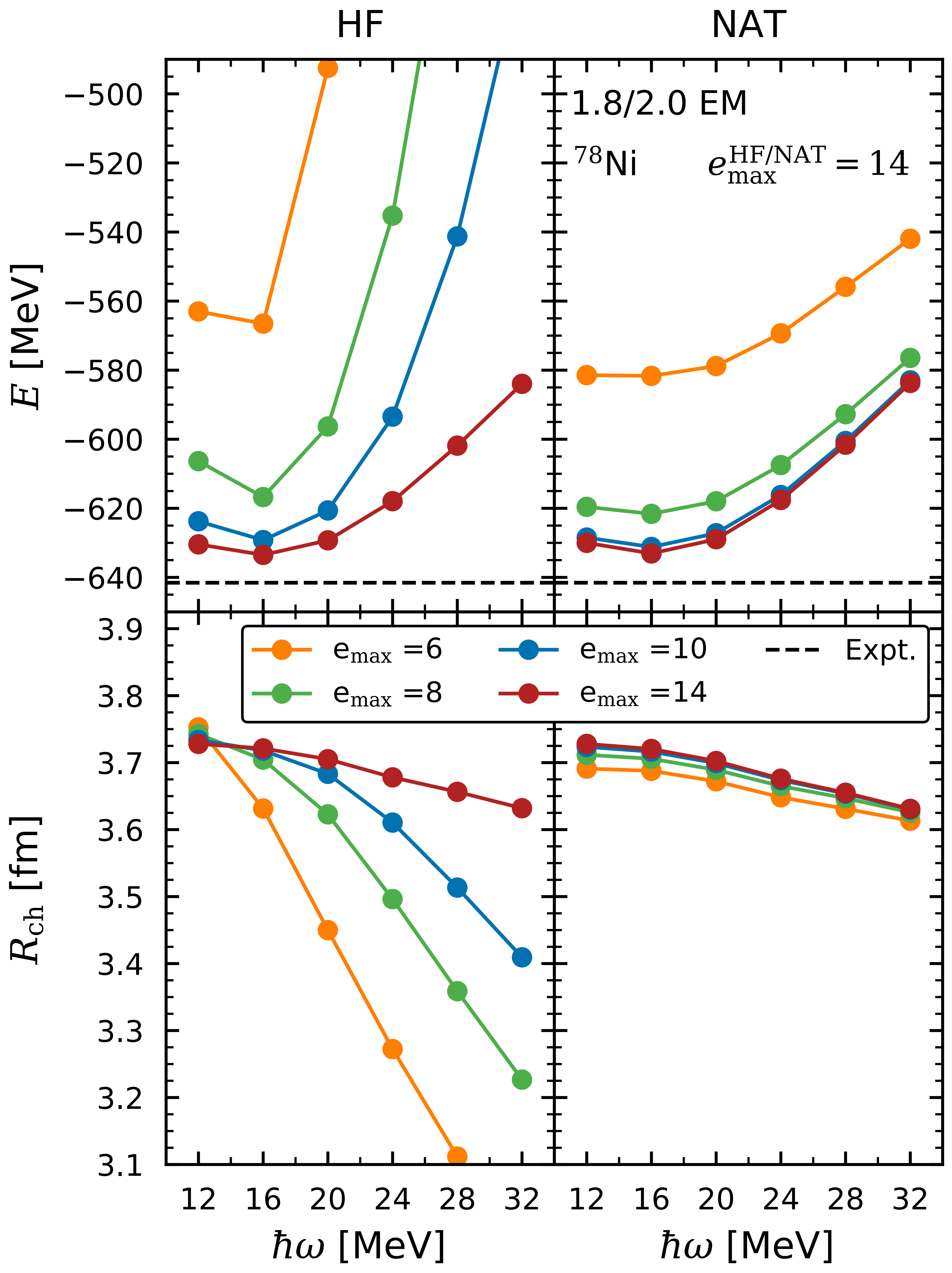
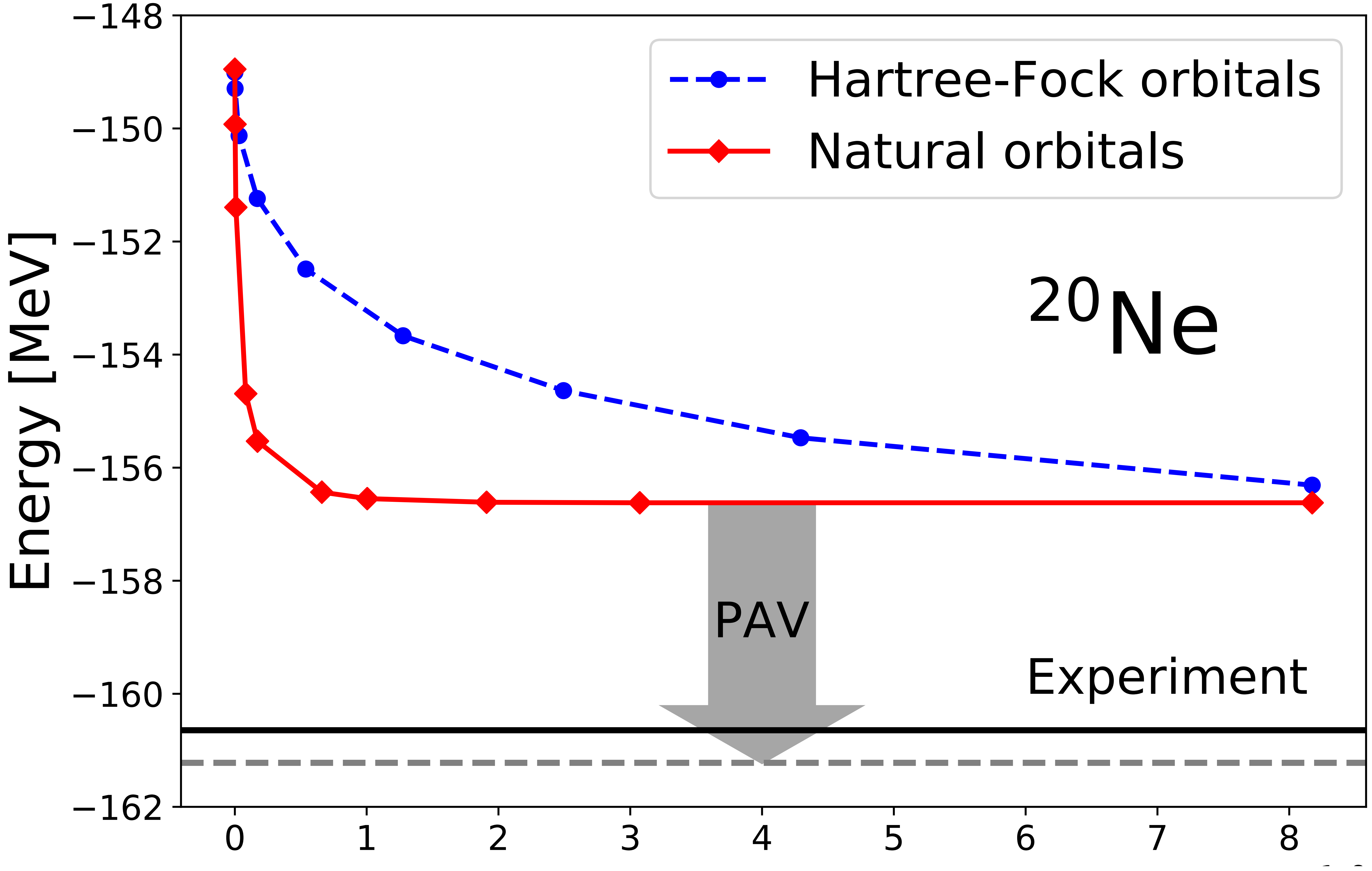


Hoppe et al., PRC **103** (2021)

Faster convergence

- NAT basis can reduce cost by a factor 10!
- ^{20}Ne is deformed
  → expensive to compute

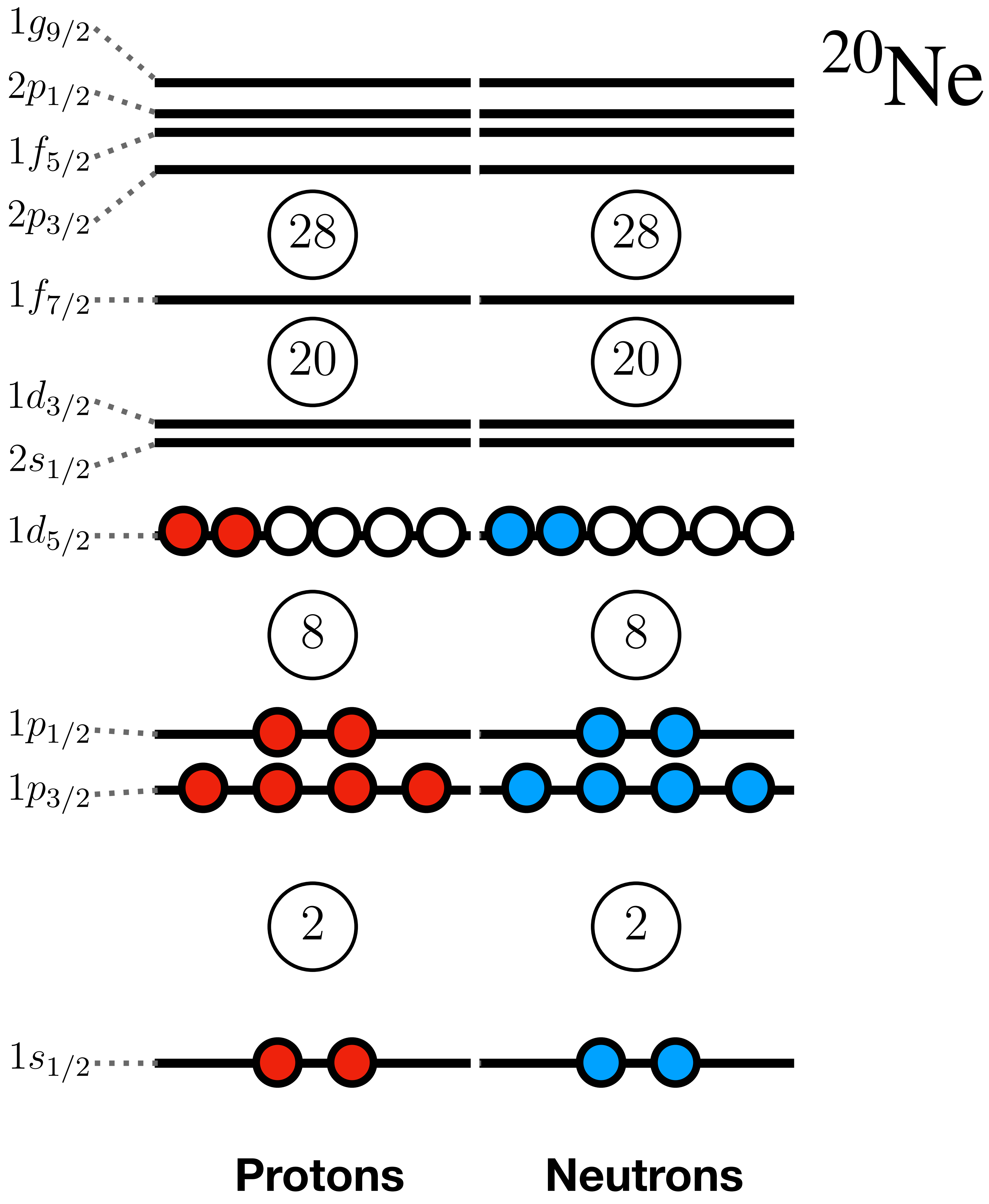


Basis size (matrix elements $\times 10^8$)

Novario et al., PRC **102** (2020)

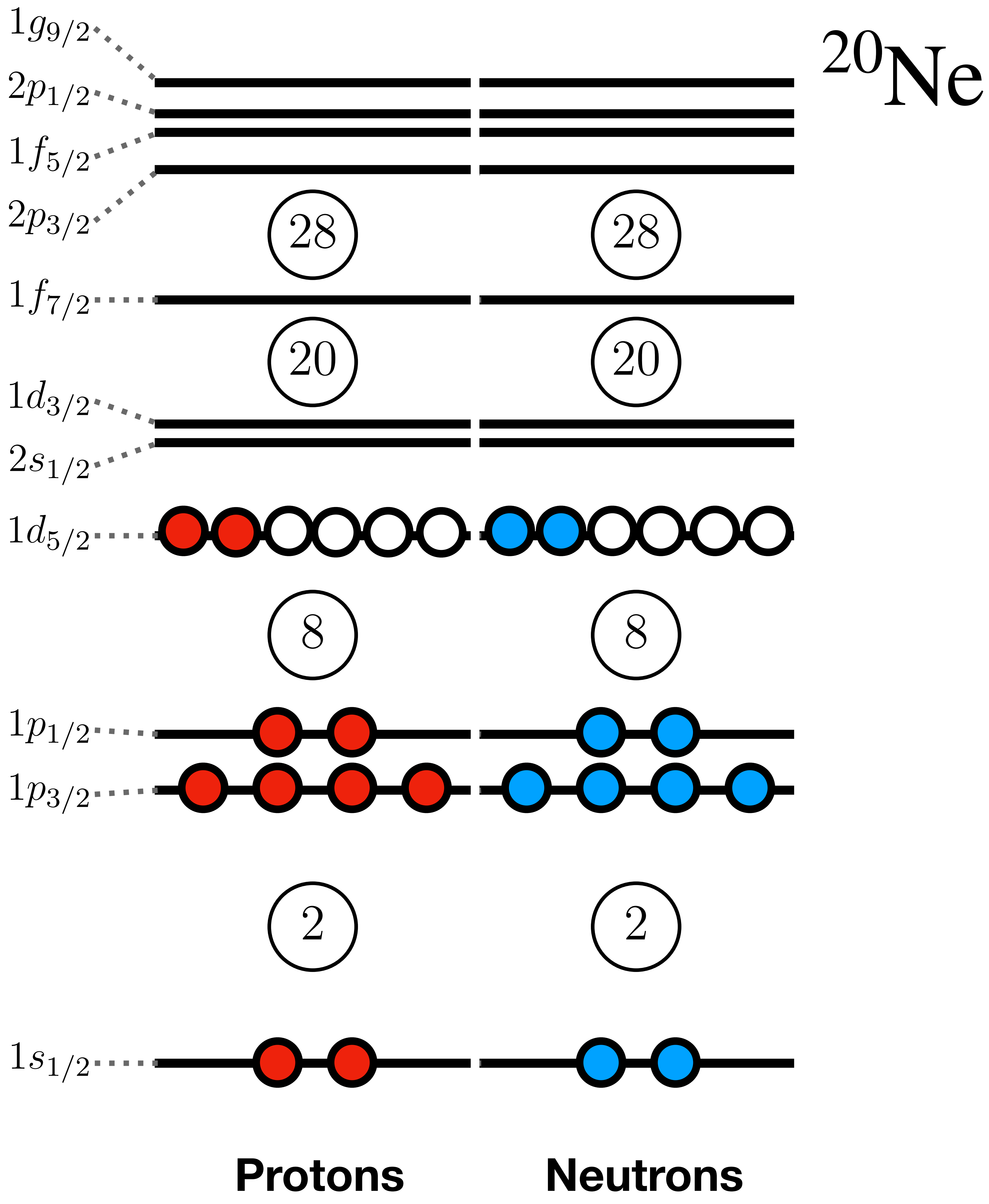
Deformed nuclei from HF

Deformation: Reference state problem



- Spherical occupation filling is not unique
- Any choice of spherical $|\Phi_{\mathrm{HF}}\rangle$ has **0-energy excitations**
  - $\rightarrow$ no reasonable perturbative expansion around $|\Phi_{\mathrm{HF}}\rangle$

Deformation: Reference state problem



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- What is wrong in our picture?
- Deformation lifts degeneracy in $m_j = j_z$

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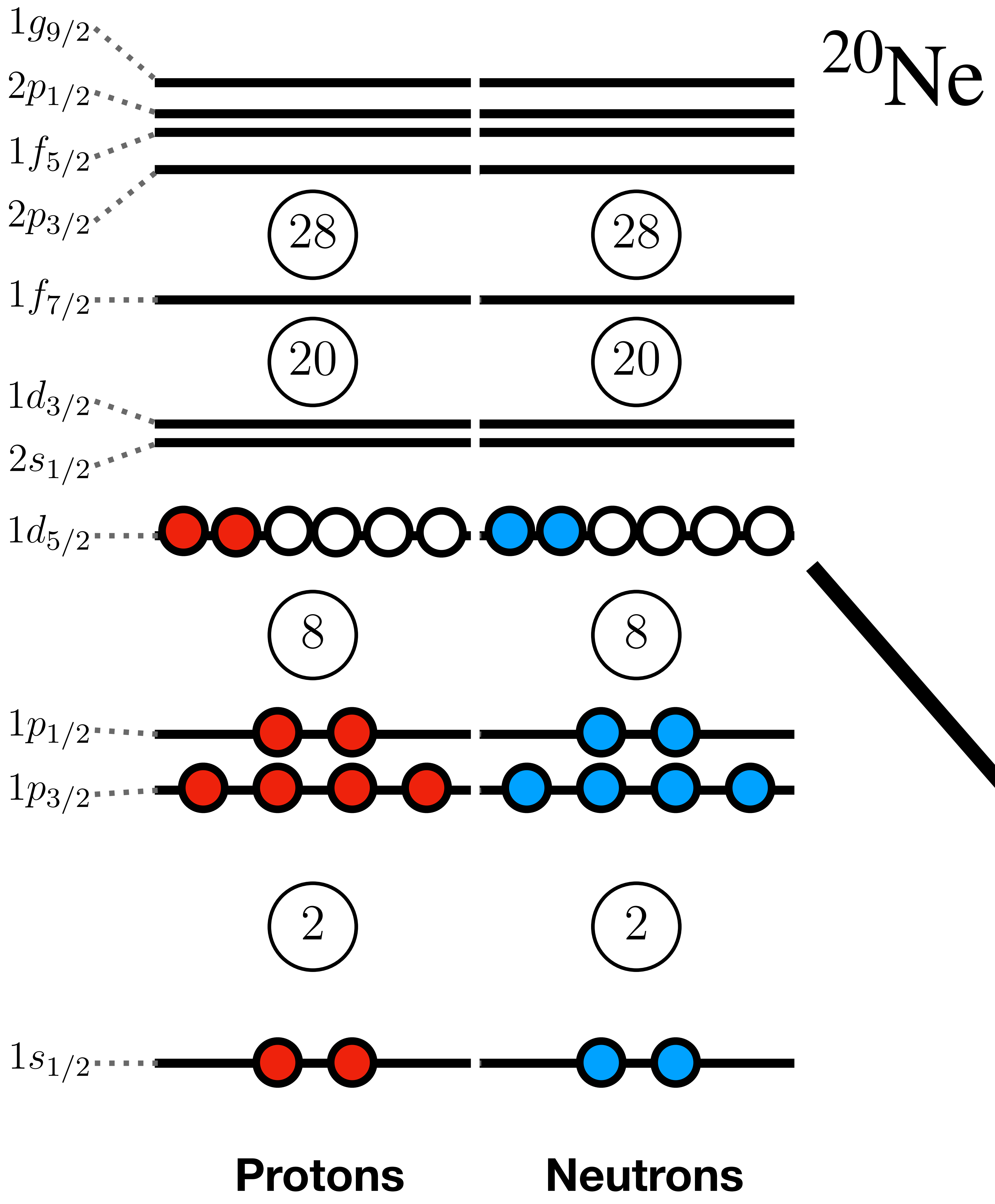

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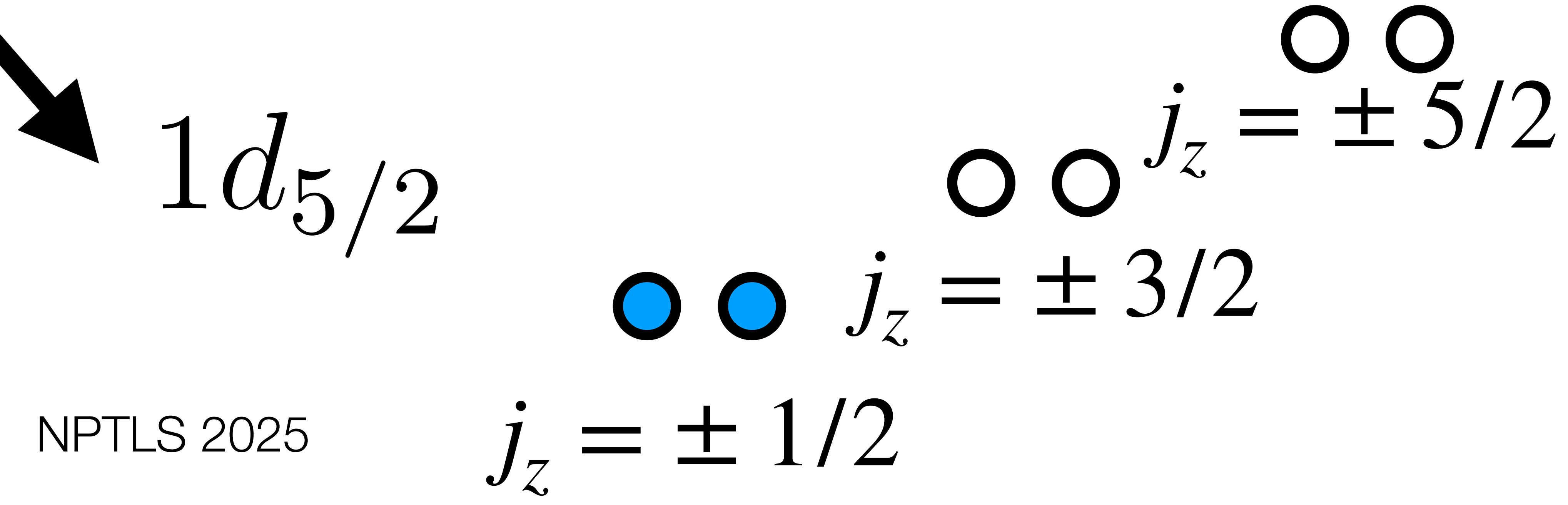


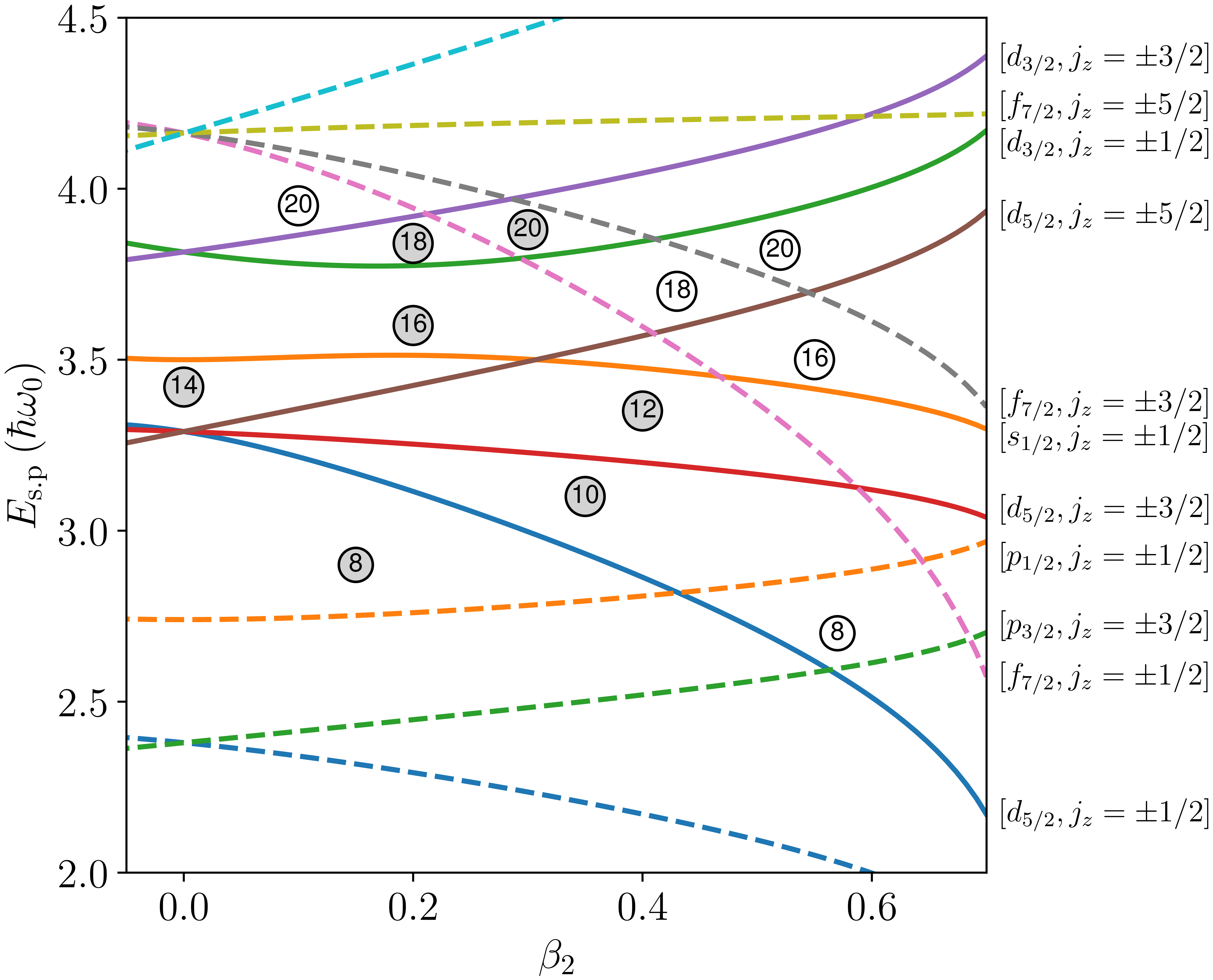
Nilsson (1955)

Nilsson model for deformation

- Axially symmetric harmonic oscillator

$$H = \frac{1}{2} m\omega_z^2 z^2 + \frac{1}{2} m\omega_\perp^2 (x^2 + y^2) + \ldots$$

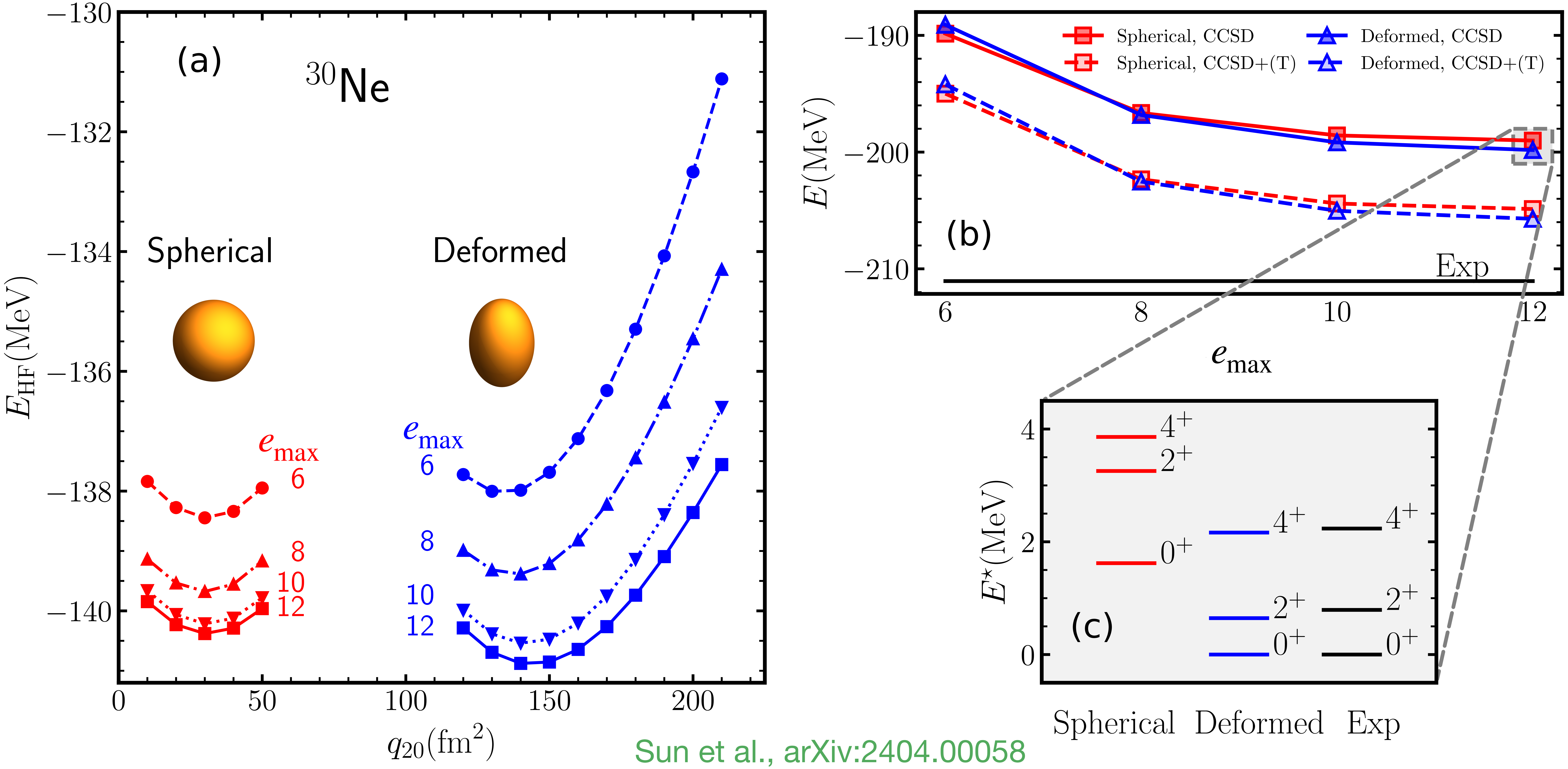
- Nucleus can be stretched or squished in z direction
- Stretched = prolate
  - $\beta_2 > 0$, mass quadrupole $Q_{20} > 0$
- Squished = oblate
  - $\beta_2 < 0$, mass quadrupole $Q_{20} < 0$



Sun et al., arXiv:2409.02279

Deformed HF guides the way

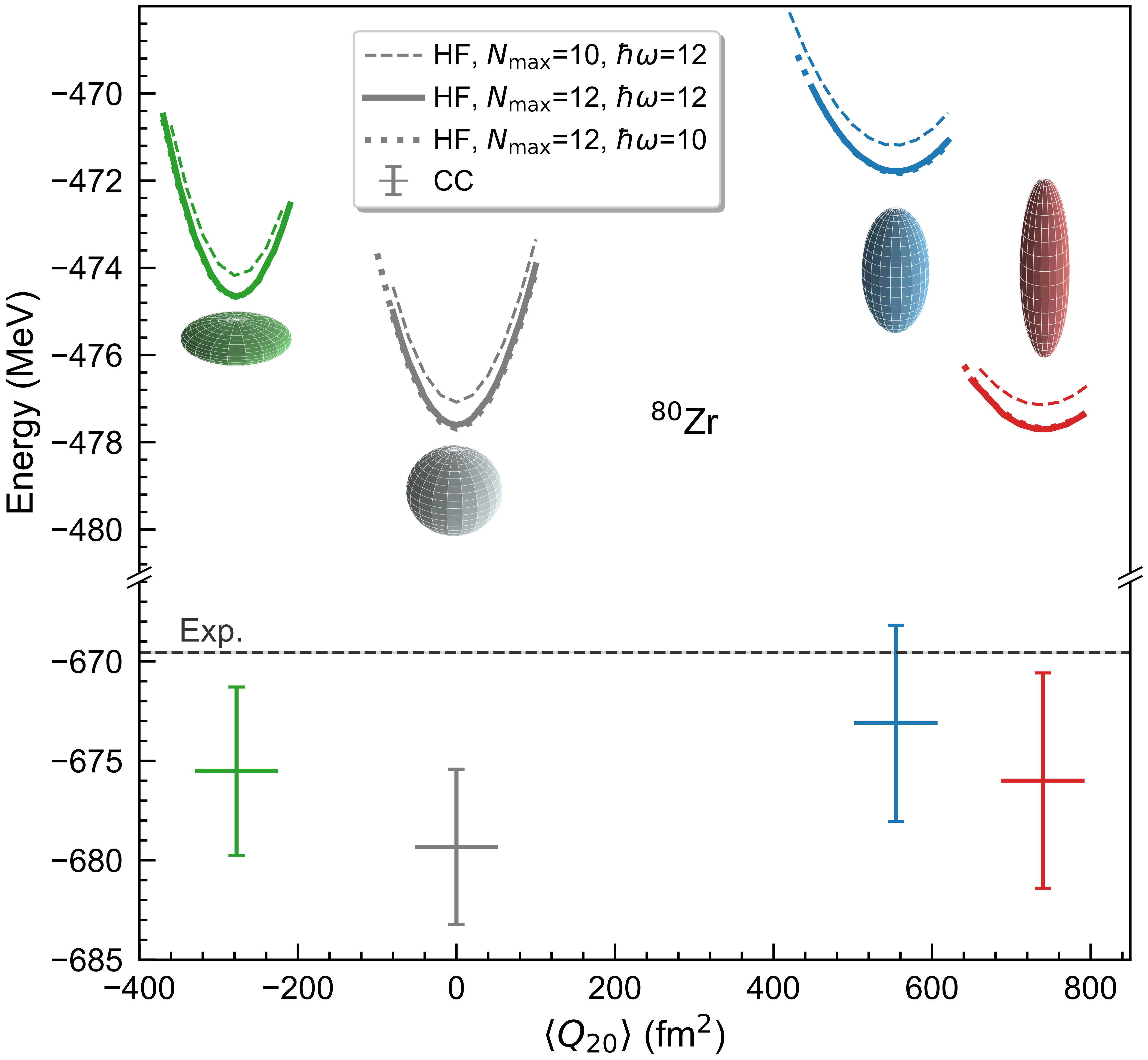
HF finds the best state with lowest energy→ tells us what deformation is preferred



Sun et al., arXiv:2404.00058

Hamaker et al., Nat. Phys. **17** (2021)

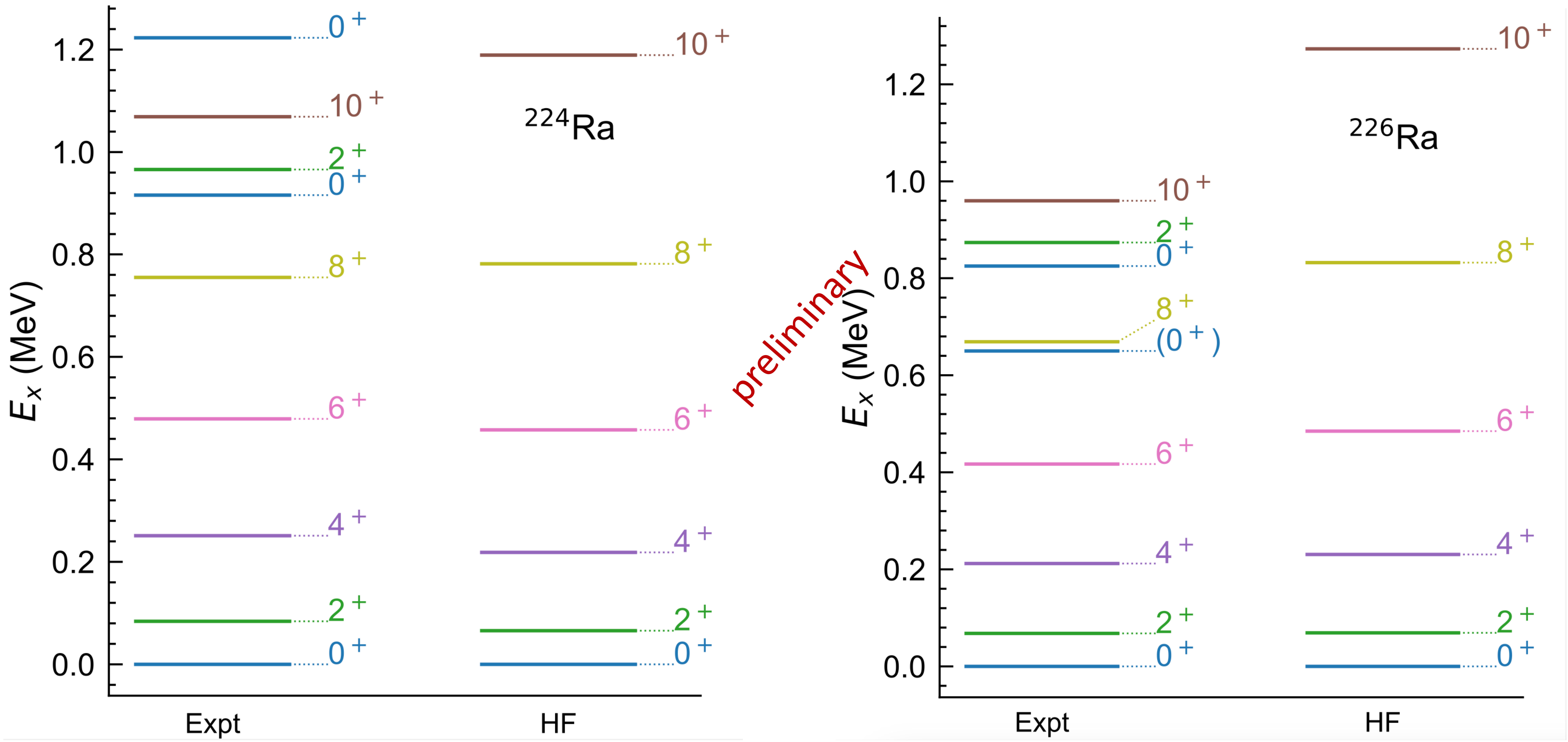
The case of ^{80}Zr



Hu et al., PRC **110** (2024)

Hu et al., preliminary

Octupole deformation in radium



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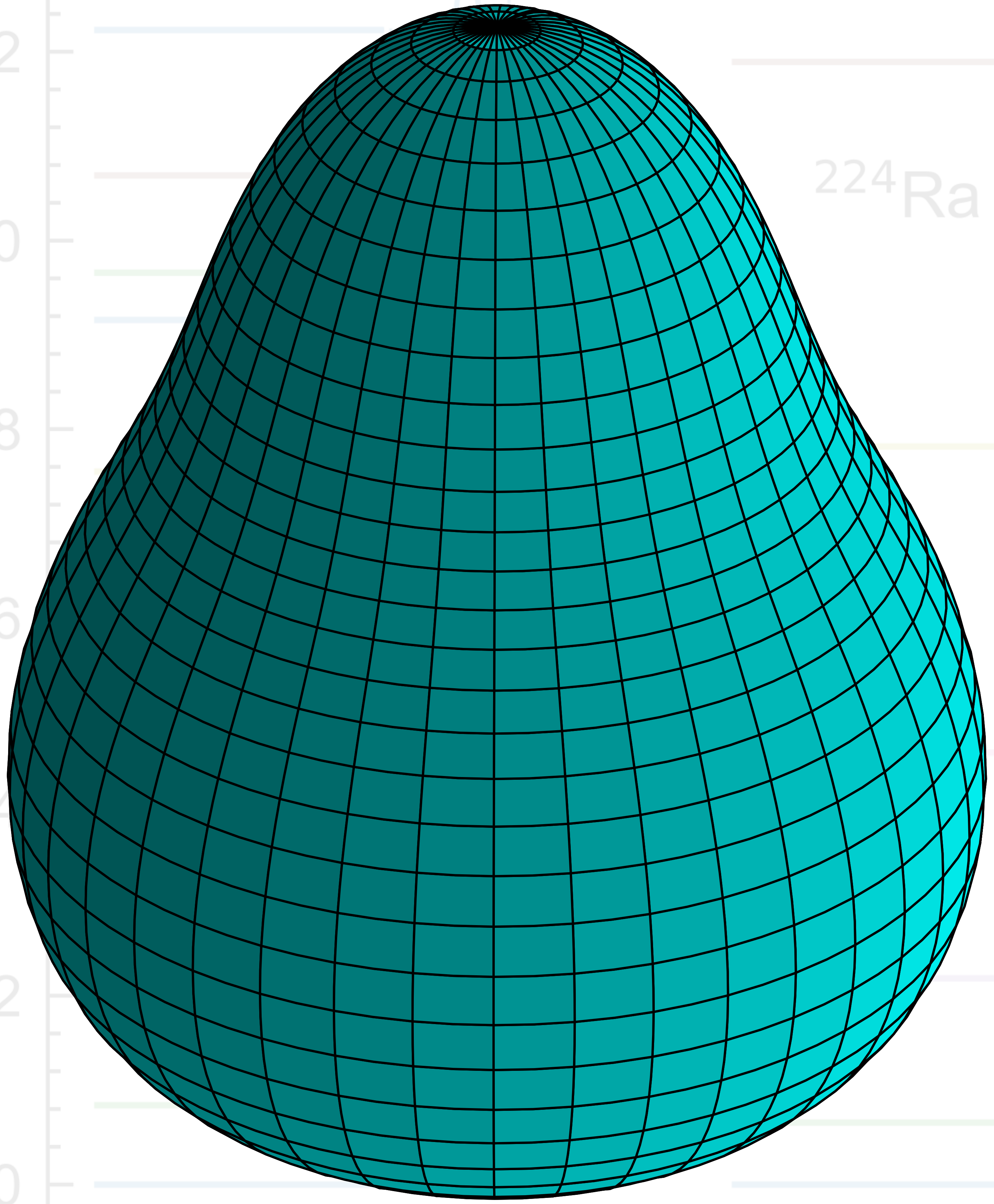

- Radium is octupole deformed
- Need to constrain multiple mass moments of nucleus
  - $Q_{10} = 0$ (center of mass!)
  - $Q_{20} > 0$
  - $Q_{30} > 0$ (octupole moment)

Conclusions

- Ab initio calculations are **challenging**, **ambitious**, slowly becoming affordable
- HF is a very important step
- **The mean field guides the way**, picks lowest energy state, informs us about deformation and other broken symmetries

Acknowledgments

Valuable references provided by:

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